

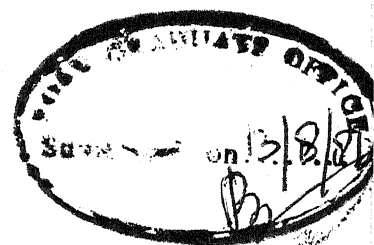
RELATIVE GAIN ANALYSIS OF ANAEROBIC DIGESTION PROCESS FOR MULTIVARIABLE CONTROL

A Thesis Submitted
In Partial Fulfilment of the Requirements
for the Degree of
MASTER OF TECHNOLOGY

by
A. K. NARESH

to the
**DEPARTMENT OF CHEMICAL ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY KANPUR
AUGUST, 1986**

CERTIFICATE



This is to certify that the present work "Relative Gain Analysis of Anaerobic Digestion Process for Multivariable Control" has been carried out by Shri A.K. Naresh under my supervision and it has not been submitted elsewhere for a degree.

Ashok Khanna
Ashok Khanna
Lecturer

August, 1986

Department of Chemical Engineering
Indian Institute of Technology
Kanpur

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- A.K. NARESH

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NOMENCLATURE

A	=	concentration of anions other than HCO_3^- , CO_3^{2-} , S^- and OH^- , eq./liter
C	=	concentration of cations other than the hydrogen ions, eq./liter
C_X	=	organism concentration, moles/liter
C_S	=	substrate concentration, moles/liter
C_C	=	$(\text{CO}_2)_D$ = concentration of dissolved CO_2 , moles/liter
$(\text{CO}_2)_D^*$	=	concentration of dissolved CO_2 in liquid phase equilibrium with the gas phase, moles/liter
C_Z	=	net cation concentration, C-A, moles/liter
C_T	=	concentration of toxic components, moles/liter
C_H	=	(HCO_3^-) = bicarbonate concentration, moles/liter
C_S^-	=	ionised substrate concentration, moles/liter
C_{SS}	=	steady state changes in the n controlled variables
D_{ij}	=	average dynamic gain between C_i and m_j
H^+	=	hydrogen ion concentration, moles/liter
K	=	Henry's law constant, moles/atm-liter
\underline{K}	=	n x n steady state process gain matrix
K_a	=	ionisation constant for volatile acid, moles/liter
K_i	=	inhibitor constant, moles/liter
K_1	=	ionisation constant for bicarbonate, moles/liter
K_{La}	=	gas transfer coefficient, day^{-1}
K_S	=	saturation constant, moles/liter
\underline{m}_{SS}	=	steady state changes in the 'n' manipulated variables
pH	=	negative logarithm to base 10 of H^+

P_C	=	partial pressure of CO_2 in the gas phase, atm
Q	=	total dry gas flow rate, $Q_{CH_4} + Q_{CO_2}$, liter/day
Q_{CH_4}	=	rate of methane production, $S_P V S_{M_X} C_X$, liter/day
Q_{CO_2}	=	Rate of CO_2 production, $-S_P V T_G$, liter/day
R_B	=	biological production rate of CO_2 , moles/liter-day
R_C	=	chemical production rate of CO_2 , moles/liter-day
RGA	=	relative gain array
RDA	=	relative dynamic array
T_G	=	gas transfer rate, moles/liter-day
V	=	reactor liquid volume, liter
V_G	=	reactor gas volume, liter
S_P	=	conversion factor, liter of gas/mole of gas
S_{C_X}	=	carbon dioxide yield, moles CO_2 produced/mole organism produced
S_{M_X}	=	methane yield, moles methane produced/mole organism produced
S_{X_S}	=	organism yield, moles organism produced/mole of substrate consumed
C_{H_3}	=	unionised substrate concentration, moles/liter
t	=	time, days
t_L	=	timelag, days
o	=	subscript indicating reactor influent
μ	=	specific growth rate, day^{-1}
μ_m	=	maximum specific growth rate, day^{-1}
θ	=	largest time constant in the process transfer function matrix
λ_{ij}	=	relative gain between i^{th} controlled variable, C_i and j^{th} manipulated variable, m_j
Λ	=	$n \times n$ relative gain array of $[\lambda_{ij}]$
ϕ_{ij}	=	dynamic potential between C_i and m_j

ABSTRACT

The relative gain method of process interaction was used for the purpose of developing new control strategies for an anaerobic digestion process, using the Andrews and Graef's model. This is done considering both the steady state and dynamic approaches. Recent developments like inclusion of timelag in growth rate function and inhibition due to toxic substances are incorporated in the model. The relative gain analysis is done around multiple steady states for different hydraulic and toxic loadings, the excess of these could result in the failure of a digester.

The results got from the analysis confirm the present day control practice and pave way to explore better control possibilities.

Chapter 1

INTRODUCTION

Anaerobic digestion, a traditional biological process for treatment and disposal of organic wastes, is receiving new and intense attention due to its simplicity and a potential to produce combustible gases. In the quest for an alternative energy source, a system encompassing energy production while controlling the environmental pollution will always be preferred. The anaerobic digestion process has gained widespread acceptance in this respect.

However, these attributes have been clouded by the misconception that anaerobic digestion tends to be an instable process. Actually, in many cases of reported instability, the difficulties have resulted from faulty operational procedures. The present day operational practise consists only of sets of empirical rules. Hence it was felt that a more rational control strategy to put the process operation on a quantitative basis, is needed.

For the purpose of quantifying the process and developing a control strategy, the steady state and dynamic relative gain method of process interactions is used. The analysis is done using the Andrews and Graef's⁴ model, where in recent developments like inclusion of timelag in growth rate function and inhibition due to toxic substances are incorporated. The analysis is carried out for different values of

the disturbance variables to make the control strategy suitable for all types of overloadings, the occurrence of which results in the failure of the digester.

Chapter 2

LITERATURE SURVEY

Scientific interest in the gas produced by decomposing animal and vegetable materials goes back to the early scientific revolution in the writings of Robert Boyle and his assistant Denis Papin in 1682. Volta in 1776 is given credit for first identifying this gas, as he found 'combustible air' to be generated everywhere in the neighbourhood of decomposing vegetation. William Henry in 1806 showed that this gas was identical with the synthetic burning gas, which was later called methane. However only in the early twentieth century, methanogenesis was found to be connected with microbial activity. From then onwards the science of methane production during digestion started developing slowly. Today the anaerobic digestion process is considered not only as a possible means of recovering energy in the form of methane gas but also in reducing the pollution load of organic wastes. The anaerobic digestion process is used widely for treating municipal waste sludge and industrial wastes containing high concentrations of organic materials. It has several significant advantages over other methods like aerobic digestion, activated sludge for the treatment of organic sludges. Other than the generation of methane gas, it forms a useful by-product in a humus-like slurry that is well suited for land reclamation.¹ Unfortunately, even with all of these advantages, reports on

the application of the process for waste treatment have indicated difficulties with process stability.

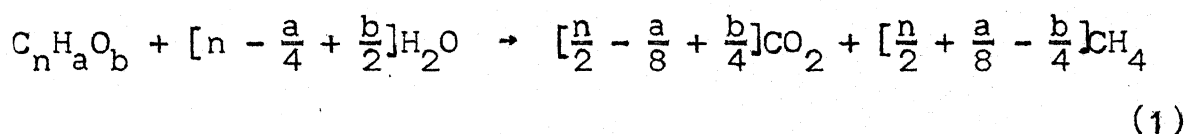
Actually, in many cases of reported instability, the difficulties have resulted from inadequate or faulty operating procedures.^{2,3} This is shown by its more successful performance in large waste treatment plants which have technical and personnel resources necessary for proper operation. The classical approach of the sanitary engineer has been to operate the process based on a set of empirical rules and the simplest steady state models. As the potentials of the anaerobic digestion process become more and more evident, there arises a great need for a more rational control strategy to put process operation on a quantitative basis. An exhaustive evaluation of process stability and control strategies for an anaerobic digester could entail years of effort if performed on a large scale. The tools of system analysis such as modelling and simulation, can reduce the time required for such a study and can be of considerable value in evaluating the effectiveness of different control strategies. They could also be of value in improving process design since it would allow comparison of the different versions of the process with respect to process stability.

Most models which are used to describe the process are steady state models and therefore cannot be used to predict process performance during start-up operations or under transient conditions resulting from changes in process inputs. A dynamic model is called for in this instance, to describe the process.

Usually the anaerobic digestion process is described as a series of reactions, where the insoluble organics are converted by the action of extracellular enzymes into soluble organics. These are changed by the action of acid producing bacteria into volatile acids. These are finally converted into methane and carbon dioxide by the methane producing bacteria. All these three steps can occur either in one reactor or the production of volatile acids can occur in one reactor and the methane production in the second reactor.

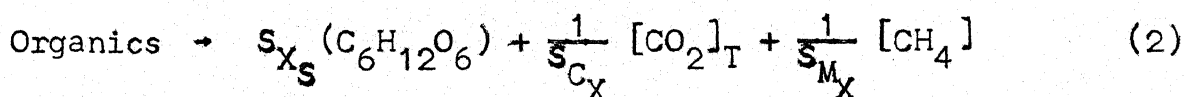
2.1 Development of the Model

Buswell and coworkers⁴ were among the first to study the anaerobic decomposition of many organic materials. They presented a general formula for the conversion of complex organic materials to carbon dioxide and methane.



However this formula does not include the fraction of substrate that is converted to microorganisms, which, though small, is necessary for the development of dynamic model of the process.

A more general formula for the conversion of organic material to microorganisms, carbondioxide is shown below^{5,6}



where,

S_{X_S} = organism yield, moles of organisms produced/mole of substrate consumed.

S_{C_X} = carbon dioxide yield, moles of CO_2 produced/mole of organisms produced.

S_{M_X} = methane yield, moles of CH_4 produced/mole of organism produced.

The values of S_{X_S} , S_{C_X} and S_{M_X} can be got from data of Lawrence and McCarty.⁴

Acetic acid accounts for approximately seventy percent of the methane produced in anaerobic digestion⁷ and the dynamic model for the digestion process is for the conversion of acetic acid to microorganisms, methane and carbon dioxide. Yields will be different for different acids, especially the increased ratio of methane to carbon dioxide produced as the length of the carbon chain of the acid increases.

Kinetics of the Process:

One of the early quantitative expressions for microbial growth was the Monod equation describing a relationship between specific growth rate and substrate concentration

$$\mu = \frac{\mu_m C_S}{K_S + C_S} \quad (3)$$

where,

μ = specific growth rate, days⁻¹

μ_m = maximum specific growth rate, day⁻¹

K_S = saturation coefficient, moles/liter

C_S = total substrate concentration, moles/liter.

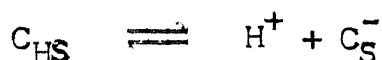
However, this Monod function cannot be valid for those substrates, such as volatile acids, that limit growth at low

concentrations and are inhibitory to the organism at higher concentrations. Andrews has proposed an inhibition function for this purpose,⁸

$$\mu = \mu_m \left[\frac{1}{1 + \frac{C_S}{K_S} + \frac{C_S}{K_i}} \right] \quad (4)$$

where, K_i = inhibition coefficient, moles/liter.

The form in which the substrate exists is also important, and Andrews has further modified the inhibition function to consider the unionised volatile acids as the limiting substrate.⁸



$$\mu = \mu_m \left[\frac{1}{1 + \frac{C_S}{C_{HS}} + \frac{C_{HS}}{K_i}} \right] \quad (5)$$

where,

C_{HS} = unionised substrate concentration, moles/liter

C_S^- = ionised substrate concentration, moles/liter

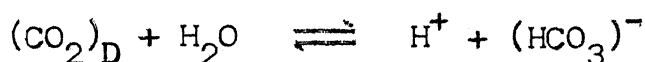
H^+ = hydrogen ion concentration, moles/liter.

For pH values above 6, the total substrate concentration, C_S , is approximately equal to the ionised substrate concentration, C_S^- . Therefore, at a fixed pH and with a known total substrate concentration, the unionised substrate concentration can be calculated from the equilibrium relationship for the substrate

$$C_{HS} = \frac{(H^+) (C_S^-)}{K_a} \quad (6)$$

where, K_a = acid dissociation constant, moles/liter.

At this stage of development, the model is restricted to a constant pH reactor and considers only two variables (pH and volatile acid concentration) important for monitoring digester operation. This restriction of constant pH was removed and the model was extended to incorporate the interaction with bicarbonate alkalinity by considering the carbon dioxide-bicarbonate equilibrium.



$$\text{i.e.} \quad \frac{(H^+) (HCO_3^-)}{(CO_2)_D} = \text{Constant} = K_1 \quad (7)$$

where,

$(CO_2)_D$ = dissolved carbon dioxide concentration, moles/liter

K_1 = ionisation constant for bicarbonate, moles/liter.

The bicarbonate alkalinity in the reactor is related to the substrate and net cation concentrations through a charge balance as shown in equation (8). For $pH > 6$, this charge balance is simplified to that shown in equations

$$(H^+) + (C) = (HCO_3^-) + 2(CO_3^{2-}) + (C_S^-) + (OH^-) + (A)$$

$$(C) - (A) = (HCO_3^-) + (C_S^-)$$

$$\text{or} \quad (HCO_3^-) = (C_Z - C_S^-) \quad (8)$$

where,

C = concentration of cations other than the hydrogen ion,
eq./liter

A = concentration of anions other than those shown in equation (8), eq./liter

C_Z = net cation concentration, $(C - A)$, eq./liter.

With the bicarbonate concentration now known from equation (8), the pH is calculated from equation (7) for constant values of dissolved carbon dioxide.

Equation (7) can be rewritten as

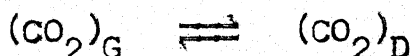
$$\frac{(H^+) (C_Z - C_S)}{C_C} = K_1 \quad (9)$$

where, $C_C = (CO_2)_D$ = dissolved carbon dioxide concentration,
moles/liter.

From equations (6) and (9), we get a relation for unionised substrate concentration

$$C_{HS} = \frac{K_1 C_C C_S}{K_a (C_Z - C_S)} \quad (10)$$

The restriction of constant dissolved carbon dioxide concentration was removed by considering the interaction between the gas and liquid phases of the reactor. At equilibrium, the dissolved carbon dioxide concentration is related to the partial pressure of carbon dioxide in the gas phase by Henry's law



$$(\text{CO}_2)_D^* = K P_C \quad (11)$$

where,

$(\text{CO}_2)_G$ = concentration of carbon dioxide in gas phase,
moles/liter of gas volume

$(\text{CO}_2)_D^*$ = concentration of dissolved carbon dioxide in the
liquid phase when in equilibrium with the gas
phase, moles/liter

P_C = partial pressure of carbon dioxide in gas phase, atm.

K = Henry's law constant, 0.024593 moles/atm-liter
at 38°C.

Under normal operating conditions, the carbon dioxide in the gas and liquid phases can be considered to be in equilibrium. However, this was not so under dynamic conditions since transfer across an interface is slow compared with ionic reaction rates. An expression for gas transfer was incorporated into the model to increase its applicability. This expression calculates the rate of transfer of carbon dioxide either to and from the liquid phase.

$$T_G = K_{La} [(\text{CO}_2)_D^* - (\text{CO}_2)_D]$$

$$\text{i.e.} \quad T_G = K_{La} [K P_C - C_C] \quad (12)$$

where,

T_G = gas transfer rate, moles/liter-day

K_{La} = gas transfer coefficient, day⁻¹.

Andrews and Graef found that in addition to hydraulic and organic loading, process failure can also be caused by

toxic materials in the feed stream to a digester.¹⁰ As a first approximation they assumed that the rate of organism kill is first order with respect to the concentration of the toxic agent as defined in equation

$$r_K = K_T C_T \quad (13)$$

where,

r_K = rate of organism kill, moles/liter/day

K_T = toxicity rate coefficient, moles of organism killed/
mole of toxic material/day

C_T = concentration of toxic material, moles/liter.

Kubicek et al. studied the effects of timelag in the specific growth function and incorporated this effect as the change in specific growth rate in the system of model equation. This was done as the microorganisms present in the sludge do not react immediately on the change of the conditions in the environment. The increase of inhibition by the substrate can also be described as increase of the timelag (delay) in the growth function. Thus we have

$$\mu = \mu_m / \left[1 + \frac{K_S}{C_{HS}(t - t_L)} + \frac{C_{HS}(t - t_L)}{K_i} \right] \quad (14)$$

Here $C_{HS}(t - t_L)$ denotes the concentration of the unionised substrate at the time $(t - t_L)$ and time t_L describes the magnitude of the timelag.

2.2 Stability of the Digester

Instability that leads to the ultimate failure of a digester can result from any material or effect that interferes

with the methane formation. The potential causes of digester instability are hydraulic, organic and toxic overloading.

This is discussed in detail in Chapter 3.

2.2.1 Process Condition Indicators

Simulation studies have evaluated the potential process condition indicators using this three types of overloading.

Total Volatile Acids:

The total volatile acids (TVA) concentration has been monitored in most digesters as an indication of the process condition of the digester. The simulations and reports from literature¹¹ indicate that a sharp rise in TVA can serve as a warning and suggest that one TVA analysis per digester per day should be adequate for routine surveillance. Nowadays, gas-liquid chromatography¹² thwarts the difficulties in on-line measurement of TVA concentration and can expedite this TVA analysis making TVA a more useful process condition indicator.

Rate of Methane Production:

This is a process variable which has not been widely used.¹³ The theory of the digestion process indicates that process condition of the digester is directly related to the rate of methane production. In all the three cases of loadings, the rate drops sharply as failure ensues, particularly in the case of toxic overloading where the rate starts to decline immediately. It is this characteristic which might enable

to sense immediately failure due to a foreign toxic substance. Another useful feature of this variable is that it can be calculated from readily available on-line gas phase measurements.

Carbon Dioxide:

Guarino et al.¹⁴ has reported the interest in the carbon dioxide content of the digester off gas for the purpose of monitoring the process. Their simulation study indicates that the carbon dioxide composition can fluctuate when the three types of loadings approach failure conditions. Carbon dioxide, the end product of the digestion process partially escapes into the gas phase and the balance either remains in solution as dissolved carbon dioxide or reacts with a base such as ammonia to form bicarbonate ions. The solubility of carbon dioxide is a function of partial pressure and the conversion of carbon dioxide to carbonates and bicarbonates depends upon partial pressure and pH.

pH:

Literature indicates that pH is a process variable that has been monitored in many digester installations to supplement information got from other process variables. Simulation studies indicate that the pH declines as the process begins to fail. This decline results from the accumulation of fatty acids and should provide an indication of changes in the condition of the process.

Other Process Variables:

Other variables that have been monitored in digestion practise to warn of process failure include total alkalinity, bicarbonate alkalinity and rate of total gas production. None of these variables were effective in predicting digester failure. However bicarbonate alkalinity would be a good indicator of digestion condition due to its relationship with the volatile acids concentration.

Kubicek et al.¹⁵ indicated that the amount of micro-organisms would be a good indicator of the digester condition and this can either be measured or the microorganism activity can be estimated from the methane gas production rate.

2.2.2 Operational Factors Affecting Stability

Andrews and Graef¹⁶ identified several factors that would add to digester stability against overloading. These included residence time, organism recycle, bicarbonate alkalinity, influent substrate concentration and frequency of loading.

Residence Time:

Increasing the residence time improves digester stability against overloading because the incoming substrate is immediately diluted to a lower concentration and provides the organisms with additional time to metabolize the substrate. The effective residence time can be increased by increasing the reactor volume and/or decreasing the reactor flow rate. The effective volume can be increased by having

additional digesters, by improving mixing to remove dead zones in the reactor or by removing grit and scum accumulations in the digester.

Bicarbonate Alkalinity:

Simulation results¹⁶ suggest that increasing bicarbonate alkalinity enables the digester to sustain sizable step increases in step loading. One way to increase bicarbonate alkalinity is by adding a base. Another way, is by increasing the influent sludge concentration to the digester. However, a sludge that is too highly concentrated can, through protein degradation, release inhibitory levels of ammonia.^{17,18} So most sludges should be concentrated to increase bicarbonate alkalinity without yielding detrimental concentrations of ammonia.

Influent Substrate Concentration:

Simulation results indicated that a concentrated influent sludge is more beneficial to digester stability than a dilute sludge. A concentrated sludge feed yields a higher steady state organism concentration within the digester, thus enabling it to sustain a larger increase in organic loading.

Digested Sludge Return:

Stability can be gained by providing sludge recycle for digesters. This is usually done by various methods — recycling a portion of digested sludge to the reactor,¹⁹ by inoculating a digester with well digested sludge from another

reactor or by degasifying and concentrating sludge in a solid-liquid separator followed by return to the digester.²⁰ Sludge return serves to inoculate the digester with additional viable organisms. Thus when overload occurs the added organism serve to increase the rate of substrate decomposition.

Loading Frequency:

Studies¹⁶ indicate that stability decreases as the frequency of loadings decrease. Certain digesters are loaded on a batch feed or discontinuous basis. The larger oscillations of the simulation variables can be substantially reduced by loading the digesters several times per day as compared to loading them once a day.

2.3 Control Strategies

Much of the earlier work on digester control has been directed towards preventing or off-setting failure. Little work has been done toward using process control techniques to increase the organic loading rate that a digester can handle ~~on~~ to improve the final quality of digester effluent. Control actions available in anaerobic digestion include a decrease in the rate of organic loading, a temporary halt in organic loading, addition of a base such as lime and soda ash, dilution of the digester contents or the addition of well digested sludge from another digester. Andrews and Graef suggested a control action which includes scrubbing of carbon dioxide from the digester gas and subsequently recycling the gas. This provides process control by adjusting

the pH of the digester through the removal of a weak carbonic acid, in contrast to the usual practise of addition of a base. pH is the measured variable and when it deviates from its set point, all on-off controller diverts a portion of the gas into a gas scrubber where carbon dioxide is eliminated by absorption in a water spray. The scrubbed gas is then recirculated to the reactor, thus reducing the partial pressure of carbon dioxide in the gas phase. This, in turn, causes dissolved carbon dioxide to be vented from the solution phase, giving an increase in pH due to the removal of carbonic acid.

Another control strategy for prevention of failure by overloading of toxic materials is the recycling of the concentrated sludge from a second stage digester using the rate of methane production as a feedback signal.¹³ The rate of methane production can be easily calculated and would be an excellent indication of the activity of the methane bacteria that are the most sensitive and critical organisms in the digester.

These current control strategies of the digester operation are based on empirical rules evolved from practical experience. Kubicek¹⁵ suggested a need for a control system which will circumvent indirect regulation methods without being too sophisticated to remain practical.

Chapter 3

CHARACTERISTICS OF ANAEROBIC DIGESTION PROCESS

3.1 Dynamic Model of the Process

The final equations representing the dynamic model for the process are now presented by approximating anaerobic digesters as continuous flow, stirred tank reactors (CFSTR) and by making material balances on the appropriate components.

The general form of a material balance is as follows:

$$\begin{aligned} &\text{Rate of material flow into reactor} + \text{Rate of appearance or disappearance of material due to reaction} \\ &= \text{Rate of material flow out of reactor} + \text{Rate of accumulation of material in reactor} \end{aligned}$$

For a multi-phase process such as anaerobic digestion it may be necessary to make material balances for specific components in each phase as well as to consider transfer of the components between phases.

(a) The mass balance for the organism

$$V \frac{dC_X}{dt} = F(C_{X_0} - C_X) + C_X \cdot V - K_T C_T \cdot V \quad (15)$$

where,

F = liquid flow rate, liters/day

V = liquid volume of reactor, liters

0 = subscript indicating influent concentration.

(b) The material balance for the total substrate is:

$$V \frac{dC_S}{dt} = F(C_{S_0} - C_S) - \frac{C_X}{S_{X_r}} \quad (16)$$

- (c) Mass balance on carbon dioxide dissolved in the solution phase

$$V \frac{dC_C}{dt} = F(C_{C_0} - C_C) + R_B \cdot V + R_C \cdot V + T_G \cdot V$$

$$R_B = C_X S_{C_X} \quad (17)$$

$$R_C = \frac{F}{V} [C_{H_0} - C_H] + \frac{dC_S}{dt} - \frac{dC_Z}{dt}$$

- (d) Gas phase carbon dioxide balance

$$\frac{dP_C}{dt} = -P S_P \frac{V}{V_G} \cdot T_G - \frac{P_C}{V_G} Q \quad (18)$$

- (e) Net cation balance

$$V \frac{dC_Z}{dt} = F(C_{Z_0} - C_Z) \quad (19)$$

- (f) Net toxic chemicals balance

$$V \frac{dC_T}{dt} = F(C_{T_0} - C_T) \quad (20)$$

The model of a digester and the information flow are indicated in Figure 3.1.

3.2 Parametric Uncertainties

The dynamic model of the digestion process consists of several parameters like K_S , K_{La} , K_1 , K_i , K_a and K . There exists an uncertainty in the value of certain parameter like K_S , K_i and K_{La} , because they are difficult to be estimated. Other parameters are 'certain' or their values are known precisely. Uncertainty arises due to the conditions

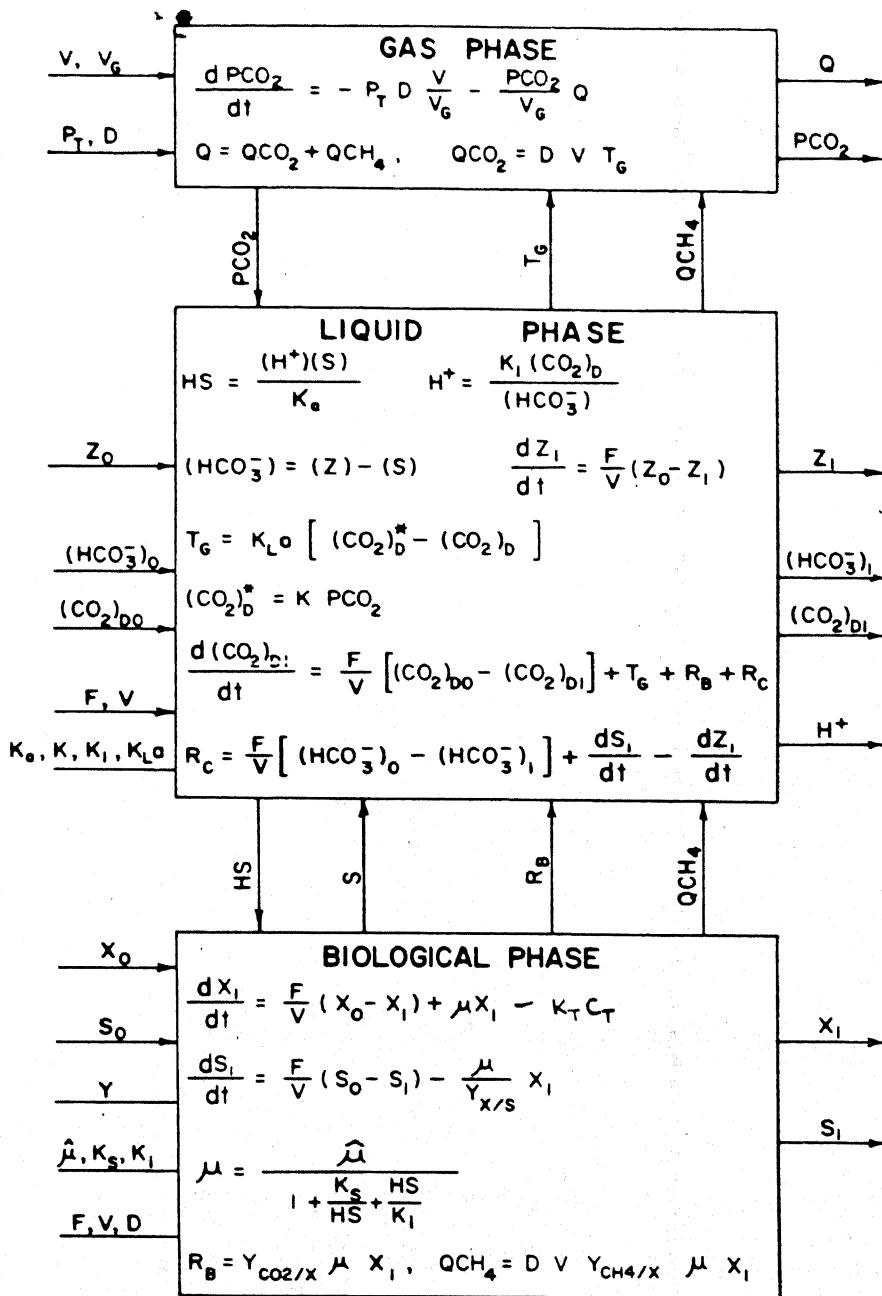


Fig. 3.1. Andrews and Graef's Model and

of the environment-temperature, concentration and composition of substrate.

Saturation Constant K_S :

There is an uncertainty in the value of K_S . K_S used to be expressed in concentrations of volatile fatty acids but it is now expressed in terms of the limiting substrate, the unionised acid. This unionised acid is dependent on an accurate knowledge of pH. Therefore K_S is very difficult to be estimated. The value of saturation constant used is

$$K_S = 0.333 \times 10^{-4} \text{ mol/lit at } 38^\circ\text{C.}^{15}$$

Gas Transfer Coefficient, K_{La} :

The values of gas transfer coefficient are not available for anaerobic digester. The model representing the system is stiff for high values of K_{La} . However, for the values of $K_{La} > 10$, the results practically do not depend on the value of K_{La} as the liquid and the gas phases are in equilibrium. The value of K_{La} used here is 30/day.¹⁵

Inhibition Constant, K_i :

Like K_S , there is an uncertainty in the value of K_i . K_i used to be expressed in concentrations of volatile fatty acids. Now, unionized fatty acids are found to be the limiting substrate and hence K_i is expressed in terms of unionised fatty acids. The unionised fatty acids are very difficult to be estimated and this causes the uncertainty in K_i . K_i is dependent on temperature, concentration

and composition of the substrate. This dependence, however, is not yet quantified. Although values of K_i for different volatile acids are not available, there is some evidence that some volatile acids are more inhibitory than others. Buswell and Morgan²¹ showed that a digester works better with a single substrate acetic acid than with both acetic and propionic acid. Venkobachar²² indicates that by properly monitoring the conditions of the environment a higher fatty acid like lactic acid can not only be less inhibitory but can also lead to higher methane production rates.

The value of K_i used here is 1.0×10^{-5} mol/lit.¹⁵

Ionisation Constant for Fatty Acids, K_a :

The value of K_a is certain and can be determined. K_a depends upon temperature, composition and concentration of the substrate. However, K_a for lower fatty acids does not seem to change appreciably with temperature. Here K_a used is 0.316×10^{-4} moles/lit.

Ionisation Constant for Bicarbonate, K_1 :

The value of K_1 is certain and can be determined. The value of K_1 used here is 0.1×10^{-5} mol/lit.

Henry's Law Constant, K :

Henry's law constant K , too is certain and can be determined. The value of K used here is 0.024593 mol/atm-lit.

The average value of the parameters K_s , K_a , K_i and yields S_{M_X} and S_{C_X} for acetic, propionic and butyric acid are given in Table 3.1.

Table 3.1

Average Values of the Parameters for Acetic, Propionic and Butyric Acids

	<u>Parameter</u>	<u>Acetic acid</u>	<u>Propionic acid</u>	<u>Butyric acid</u>
(1)	K_s (mg/lit) 35°C	154	32	5
(2)	K_i (mol/lit) 38°C	1.0×10^{-5}	-	-
(3)	K_i (mol/lit) 35°C	$10^{-4.56}$	$10^{-4.7}$	$10^{-4.82}$
(4)	S_{M_X}	47.0	47.0	80.0
(5)	S_{C_X}	47.0	47.0	47.0

The values of parameters used by Andrews and Graef are given in Table 3.2.

3.3 Multiplicity of Solutions

Andrews and Graef in their dynamic simulations obtained two steady state solutions. One of them stable and the other unstable, by varying certain parameters in their model. Kubicek et al.¹⁵ found in a certain range of parameters, three steady state solutions, two of which are stable.

Multiplicity of solutions arises due to the dependency of certain parameters like K_a and K_i on composition and concentration of the substrate and temperature. The sensitivity of the stationary solutions to the individual values of parameters in certain cases is high.

The dependences of the stationary values of substrate concentration on volatile acid dissociation constant

Table 3.2

Values of Parameters Used in Andrews and Graef Model

<u>Parameter</u>	<u>Value</u>	<u>Unit</u>	<u>Meaning</u>
F	1.0	l/day	Flow rate
K	0.024593	mol/l-atm	Henry's law constant
K _a	0.316×10^{-4}	mol/l	Acid dissociation constant
K _i	0.667×10^{-3}	mol/l	Inhibition constant
K _{La}	100	day ⁻¹	overall gas transfer film coefficient
K ₁	0.1×10^{-5}	mol/l	Ionisation constant of the bicarbonate
K _S	0.303×10^{-4}	mol/l	Saturation constant
S _{XS}	0.02	-	Organism yield
S _{CX}	47.0	-	CO ₂ yield
S _{MX}	47.0	-	CH ₄ yield
V	10.0	l	Digester volume
V _G	2.0	l	Volume of gas space in the digester
μ _m	0.4	day ⁻¹	Maximum specific growth rate
p	0.93421	atm	Total pressure
K _T	2.0	day ⁻¹	Toxicity influence rate
S _P	25	l/mol	Conversion factor
C _{XO}	0.001	mol/l	Inlet concentration of organism
C _{SO}	0.09	mol/l	Inlet concentration of substrate
C _{CO}	0.009	mol/l	Inlet concentration of dissolved CO ₂
C _{ZO}	0.1	mol/l	Inlet concentration of net cation
C _{TO}	0.0	mol/l	Inlet concentration of

K_a and the stationary values of substrate and biomass concentration on inhibition constant K_i are shown in Appendix A.

The stationary or steady state solutions for the anaerobic digester were obtained numerically from the model representing the digester, by setting the derivatives in the model to zero.

The dependence of the stationary value of the substrate concentration on the value of flow rate, F for a value of $K_i = 10^{-5}$ is shown in Figure 3.2. Three stationary solutions were obtained. Of these three steady states, two of them (a and c) are found to be stable and the middle steady state (b) is found to be unstable. The reason is if we give a perturbation in any one of the manipulated variables (inlet organism concentration C_{x_0} , inlet substrate concentration C_{s_0} and inlet dissolved carbon dioxide concentration C_{c_0}), it results in the shifting of the steady state 'b' to the stable states (a and c), according to the direction of the perturbations.

Again, of the two stable steady states, the steady state corresponding to low substrate conversion (a) is found to be highly productive whereas steady state (c) corresponding to a high substrate conversion, is found to be unproductive. The reason for this is shown in Figure 3.2. The figure indicates that the rate of methane formation is very high in the steady state 'a' than compared to the steady states 'b' and 'c' and hence the best operable steady state.

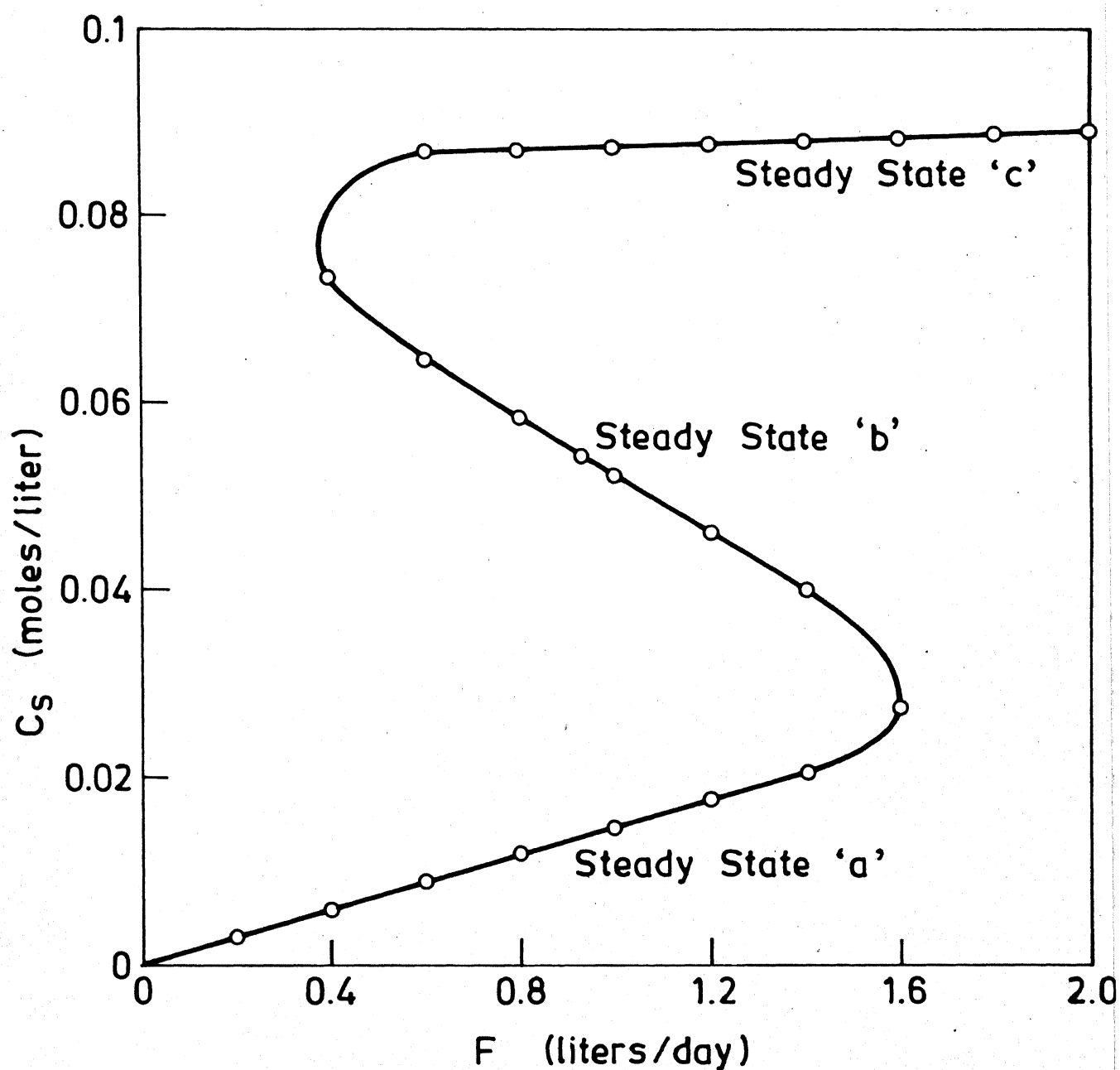


Fig. 3.2. Dependence of Stationary Solutions on the of F . $K_{La} = 30$, $K_i = 10^{-5}$, Other Parameters as in Table 3.2.

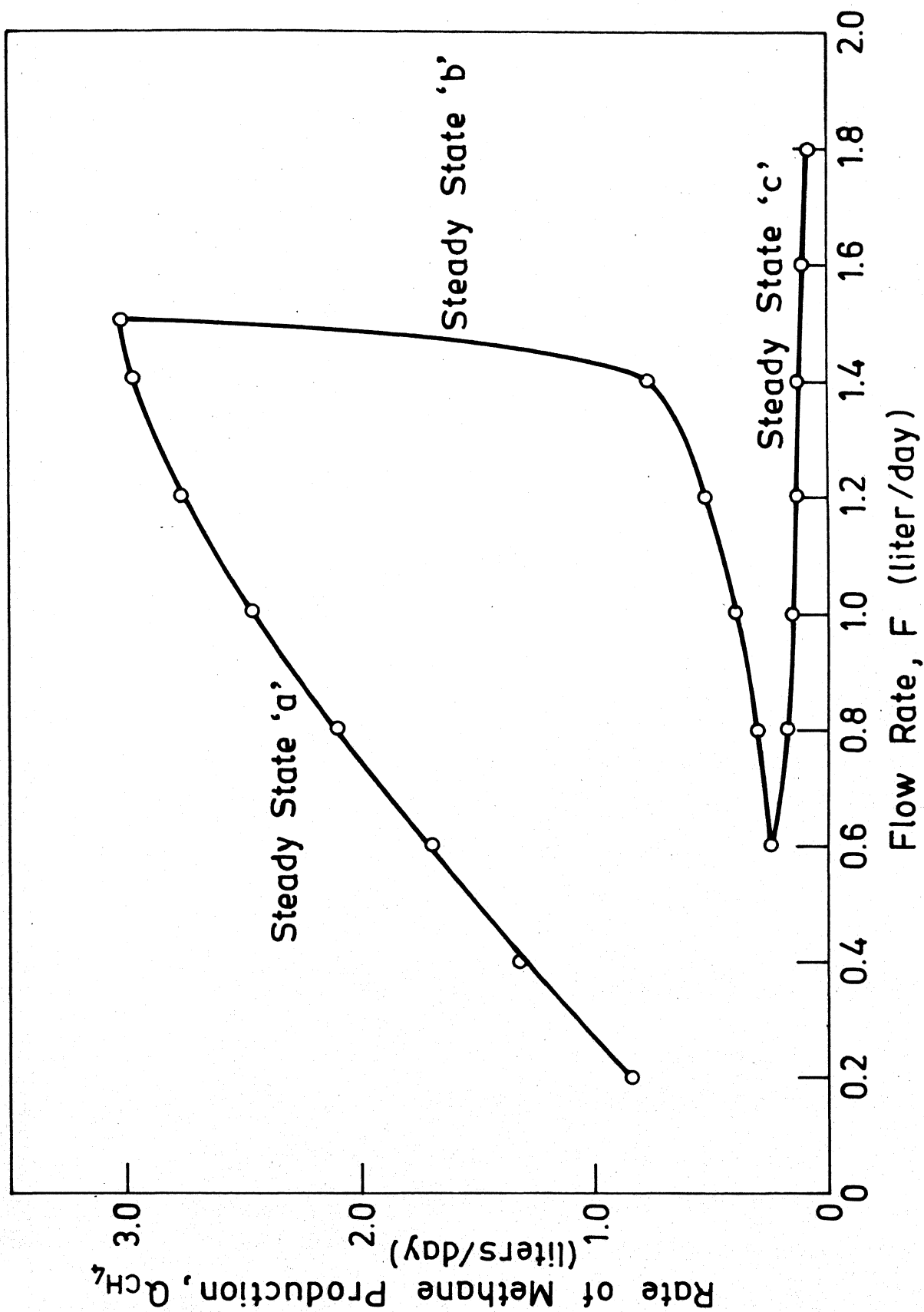


Fig. 3.3. Dependence of Rate of Methane Production, Q_{CH_4}

3.4 Digester Failure

Many cases of digester failure arise because of the operation not recognising the signs of impending difficulty. If the process variables are monitored well, it is likely that the failure can be thwarted.

In a digester, failure is due to the instability which results from any material or effect, that interferes with methane formation. Three potential causes of digester instability and ultimate failure are hydraulic, organic and toxic overloading.¹⁶

Hydraulic overloading can occur whenever there is a washout of the microorganisms. This increase in flow rate 'F' happens when sludge production exceeds design capacity or whenever too much sludge is pumped into the digester. The residence time can also be decreased if top deposits of grease and scum accumulate within the digester or when insufficient mixing produces stagnant zones in the reactor.

Organic overloading can occur whenever there is an accumulation of volatile acids in the digester, that can inhibit the methanogenic organisms. This can result whenever there is a sudden increase in organic solid feed concentration caused due to excessive digester loading (increase in flow rate 'F') or attempting to start up a digester too rapidly. Another source for failure due to organic overloading is when a carbohydrate predominant sludge is added. The decomposition of carbohydrates, in contrast to normal sludge degradation, in which ammonia is a metabolic product,

yields short chain fatty acids without the accompanying buffer action provided by ammonia. This results in the fatty acids remaining in the unionised form which are inhibitory.

Toxic overloading can occur when a material that can kill the methanogenic microorganisms is introduced. The materials that have caused failure includes heavy metals, detergents, organic chemicals, ammonia and various cations. Fortunately, this failure can be prevented as there is always sufficient dilution capacity to dilute these toxic agents occasionally found in domestic and industrial wastewaters.

Besides these three potential causes of digester instability, failure can also occur due to the effect of timelag in the specific growth function. The microorganisms present in the sludge do not react immediately to the change in conditions of the environment i.e. concentration of the substrate. The increase of inhibition by the substrate can also be described as an increase of the timelag (delay) in growth rate function. The timelag has a destabilising effect. For a sufficiently large timelag ($t_L > 2.5$ days) this effect is pronounced. Fortunately, in practise, the observed timelag is very small⁹ ($t_L = 0.3$ day) and does not pose any serious problem of destabilising the digester (Appendix A).

Chapter 4

RELATIVE GAIN ANALYSIS

The traditional industrial control strategy for multivariable control problems, where several process variables are to be controlled and several variables can be manipulated, is to use a multiloop control scheme consisting of several conventional controllers. In designing a multiloop control system, a key design decision is to determine the proper pairing of controlled and manipulated variables. If an incorrect pairing is used, the resulting control system might perform very poorly or even be inoperable depending on the level of interaction between the control loops.

To illustrate the multiloop control strategy and interaction of control loops, consider a process, which has two controlled variables C_1 and C_2 , and two manipulated variables m_1 and m_2 . There are two possible control loop configurations. One approach would be to control C_1 by adjusting m_1 and to control C_2 by adjusting m_2 . This is referred to as a 1-1/2-2 configuration. The alternative approach is to control C_1 by adjusting m_2 and to control C_2 by adjusting m_1 i.e. a 1-2/2-1 configuration.

Let us take 1-1/2-2 configuration. To understand the nature of interaction between two control loops, the effect of input changes or the outputs is studied when

- (i) One loop is closed and the other is open, and
- (ii) Both loops are closed.

In the former case (Figure 4.1a), it is clear that any change in the set point R , sp will affect not only the behaviour of controlled output C_1 but also the uncontrolled output C_2 .

In the later case (Figure 4.1b), consider a change in set point R_1 , sp only and keep the set point R_2 , sp the same. Then controller of loop 1 will change m_1 to bring C_1 to the set point value. This is direct effect of m_1 on C_1 through loop 1.

The control action of m_1 will not only bring C_1 to set point but also disturb C_2 from steady state. To make C_2 constant, the controller of loop 2 changes appropriately the value of m_2 . But a change in m_2 in turn affects output C_1 . This is an indirect effect of m_1 on C_1 .

This constitutes the essence of effect of interaction between two control loops. For better controls, interaction between loops should be minimum.

The most prominent approach for characterising process interactions is the Relative Gain Array (RGA) method, proposed by Bristol.²³ This method, based on the steady state process model, provides useful information to categorize process interaction. However, process dynamics needs to be considered in many situations and another method, dynamic gain array method was proposed,^{25,28} which gives a useful insight into the dynamic behaviour and also provides a measure of dynamic interactions as well. By studying both the steady state and dynamic approaches, a total picture of the behaviour of the process can be got and measured.

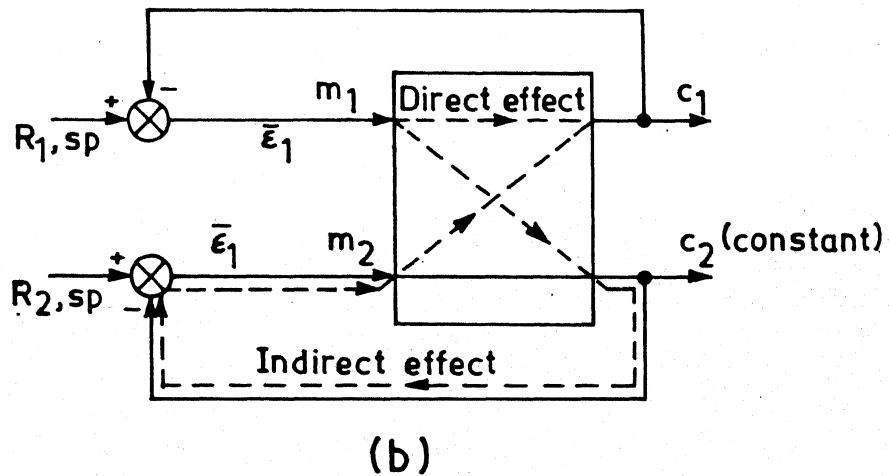
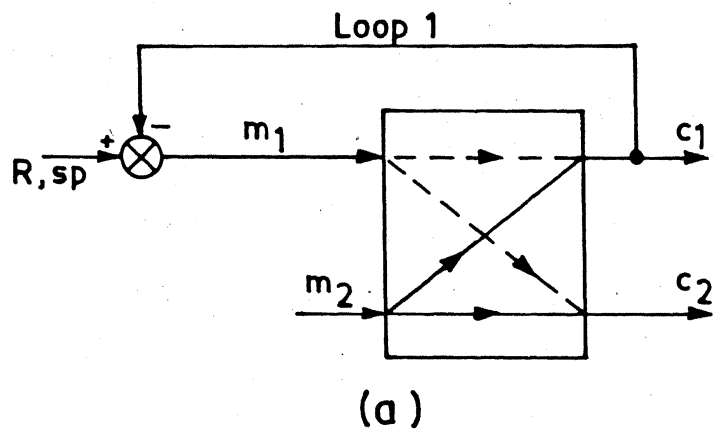


Fig. 4.1. Interactions Among Control Loops:
 (a) One Loop Closed;
 (b) Both Loops Closed.

4.1 Steady State Approach

To illustrate the relative gain array method, consider the steady state process model

$$\underline{C}_{ss} = \underline{K} \underline{m}_{ss} \quad (21)$$

where \underline{C}_{ss} and \underline{m}_{ss} are the steady state changes in the n controlled and n manipulated variables, respectively, and \underline{K} is the $n \times n$ steady state process gain matrix.

The relative gain between the i^{th} controlled variable, C_i and j^{th} manipulated variable, m_j will be denoted by λ_{ij} .

This dimensionless quantity is defined as

$$\lambda_{ij} = \frac{\text{Open loop gain}}{\text{Closed loop gain}} \quad (22)$$

Mathematically, it can be expressed as

$$\lambda_{ij} = \frac{(\partial C_i / \partial m_j)_m}{(\partial C_i / \partial m_j)_C} \quad (23)$$

In this equation, the partial derivative in the numerator is evaluated by keeping all the manipulated variables except m_j constant (Figure 4.1a). Similarly, to evaluate the partial derivative in the denominator, all of the controlled variables except C_i are held constant (Figure 4.1b). This latter condition can be achieved (in principle) by adjusting the other $n-1$ manipulated variables.

From eq. (1) it is apparent that the open loop gain between C_i and m_j is \underline{K}_{ij} , an element of the process gain matrix, \underline{K} . Bristol²³ has shown that the closed loop gain is

$1/\tilde{K}_{ij}$ where \tilde{K}_{ij} is an element of the matrix inverse of the transpose of \underline{K} .

$$\tilde{\underline{K}} = \tilde{K}_{ij} = [\underline{K}^T]^{-1} \quad (24)$$

Now, the expression for λ_{ij} becomes

$$\lambda_{ij} = \underline{K}_{ij} \tilde{K}_{ji} \quad (25)$$

The Relative Gain Array is defined to be the $n \times n$ matrix,

$$\Lambda = [\lambda_{ij}]$$

The relative gain array is a square matrix which implies that number of manipulated variables is equal to number of controlled variables.²⁴

A useful characteristic of the relative gain matrix is the fact that the sum of the λ_{ij} 's of any row or column of the matrix has a sum equal to the unity.

$$\sum_{i=1}^N \lambda_{ij} = 1 \quad \text{for } j = 1, 2, \dots, N$$

(summation by rows)

$$\sum_{j=1}^N \lambda_{ij} = 1 \quad \text{for } i = 1, 2, \dots, N$$

(summation by columns)

The relative gain gives an useful measure of interaction and provides a recommendation concerning the proper control configuration. In particular:

- (1) If $\lambda_{ij} = 0$, then manipulation of m_j has no effect on the control variable C_i .

- (2) If $0 < \lambda_{ij} < 1$, then an interaction exists and manipulation of variables other than m_j also affect the steady state value of the control variable C_i . The smaller the value of λ_{ij} , the larger the interaction.
- (3) If $\lambda_{ij} = 1$, then the control loop formed between C_i and m_j does not interact with the other loops formed between the other controlled and manipulated variables. So manipulating other variables (other than m_j) does not affect C_i .
- (4) If $\lambda_{ij} < 0$, then other manipulations (other than m_j) causes a strong effect on C_i and in a direction opposite from that caused by manipulating m_j . The interaction effect is very dangerous in this case.
- (5) If $\lambda_{ij} > 1$, then the response of the output C_i is held back by the interaction from the other loops formed between the other controlled and manipulated variables. The longer the values of the relative gain above unity, the larger will be the "holding back" effect.

Criteria for Selection of Control Loops:

From the characteristics of relative gains and relative gain array, it is seen that the best control loops (with minimum interaction) are got by pairing the controlled outputs C_i with the manipulated variables m_j in such a way that the relative gains λ_{ij} are positive and as close as possible to unity.

4.2 Dynamic Approach

Although the steady state RGA method provides useful information, it neglects the dynamics of the process. In some situations, the dynamic characteristics may be an important factor in determining the control configurations. Consequently, other measures have been proposed which includes both static and dynamic behaviour of the process.²⁵⁻²⁷

We have adopted the Witcher and McAvoy approach. Witcher and McAvoy's measure of process interaction was based on open loop step responses. This information can be got from experimental data or from transient response of a process model, for e.g., a transfer function or state space model. Thus this method is widely used as it does not require a particular type of process model.

The interaction measure is based on a 'dynamic potential' ϕ_{ij} , which is the integral of the open loop step response, $C_i(t)$ to a step change in m_j at time $t = 0$.

$$\phi_{ij}(\theta) = \int_0^{\theta} C_i(t) dt \quad (i, j = 1, 2, \dots, n) \quad (26)$$

Here the selection of θ , the time period over which the integration is performed, is somewhat arbitrary. It is specified as 20% to 100% of the dominant time constant of the process. By substituting $\phi_{ij}(\theta)$ for steady state gain K_{ij} in equation (25), Witcher and McAvoy constructed a 'Relative Dynamic Array' (RDA) with element $\lambda_{ij}(\theta)$ given by

$$\lambda_{ij}(\theta) = \phi_{ij}(\theta) \cdot \phi_j(\theta)$$

where $\phi_{ji}(\theta)$ is a element of $\phi(\theta)$ and $\phi(\theta) = \phi(\theta)^T^{-1}$.

The selection of loops in this case is similar to RGA method. However, this method has a shortcoming in that both $\lambda_{ij}(\theta)$ and the recommended pairing depend on the value of θ , which is not well defined.

A new measure of process interactions, a modified form of Witcher and McAvoy method, was proposed by Gagnepain and Seborg.²⁸

This was an extension of the RDA concept since it was also based on the open loop step responses. However, to avoid the disadvantages of the RDA method, the resulting dynamic response data are used in a different manner.

Suppose that the process is initially at steady state and that a unit step change m_j occurs at $t = 0$. During the time interval $(0, d_{ij})$, C_i is not affected by m_j and the 'dynamic gain' of the process at this time period is zero. For the time interval (d_{ij}, θ) , the average dynamic gains, D_{ij}^* , between C_i and m_j can be calculated as

$$D_{ij}^* = \frac{(\text{Average change in } C_i)}{(\text{Change in } m_j)}$$

But since, at steady state a unit step change was made in the process, it follows that D_{ij}^* is equal to the average of C_i over the time interval (d_{ij}, θ) .

$$D_{ij}^* = \frac{1}{\Delta m_j} \frac{1}{\theta - d_{ij}} \int_{d_{ij}}^{\theta} C_i(t) dt$$

A piecewise constant function is defined conveniently as

$$C_{ij}(t)$$

$$\begin{aligned}\underline{D}_{ij}(t) &= 0 && \text{for } t < d_{ij} \\ &= \underline{D}_{ij}^* && \text{for } d_{ij} \leq t \leq \Theta\end{aligned}$$

In a further modification of Witcher and McAvoy method for a process with negligible timelag, we have the average dynamic gain, \underline{D}_{ij} as

$$\underline{D}_{ij} = \frac{1}{\Delta m_j} \frac{1}{\Theta} \int_0^{\Theta} C_i(t) dt$$

where Θ is the largest time constant in the process transfer function matrix.

In analogy with RGA and RDA, average dynamic relative gain is defined in terms of $\underline{D}_{ij}(t)$

$$\mu_{ij}(t) = \underline{D}_{ij}(t) \underline{D}_{ji}(t)$$

where \underline{D}_{ji} is an element of $\underline{D} = (\underline{D}^T)^{-1}$.

Chapter 5

RESULTS AND DISCUSSION

5.1 Calibration of the Simulation Software

In order to check the consistency of the software developed we tried to reproduce the batch simulation results of Andrews and Graef⁴ using his data. Tremendous difficulty was encountered in producing this match. During this difficult period several parallel numerical techniques were tried: Powell algorithm, Brown's method and Math proton method. Continuous debugging of the program led to discovery of an error in Kubicek's model presentation.¹⁵ Dynamic equation for partial pressure of carbon dioxide carried a plus sign with the pressure term, whereas the physics of the problem indicates a minus sign.

After removal of the error indicated above, dynamic simulation was tested and confirmed with Kubicek's simulated results (Appendix B).

5.2 Steady State Analysis5.2.1 Hydraulic Loading

From the equations representing the model we have C_{X_0} , C_{S_0} , C_{C_0} as the inlet concentrations (manipulated variables), and C_X , C_S , C_C , P_C , C_Z and C_T as outlet variables. Among the outlet variables, the controlled variables are to be chosen. In the model, equations (19) and (20) have a linear first order form and $C_Z(t)$ and $C_T(t)$ are stable and

and tend to the inlet conditions C_{Z_0} and C_{T_0} . Thus, according to the model, only the first four variables C_X , C_S , C_C and P_C need to be controlled.

Of these four variables, C_S , C_C and P_C are measurable and also C_X can either be measured or microorganism activity can be estimated from the methane gas production rate. Control strategies should be developed using relative analysis such that each manipulated variable controls one controlled variable only so as to achieve a near perfect decoupling of the loops (with minimum interaction) formed between the controlled and the manipulated variable.

The current practise of digester operation involves empirical control rules using rate of methane production QCH_4 and pH as feedback control variables. Considering them among the variables to be controlled, we have 6 possible process variables to be controlled, C_X , C_S , C_C and P_C from the equations representing the model and QCH_4 and pH from current operational practise.

As mentioned earlier, flow rate 'F' is considered as a disturbance variable. Similarly C_{T_0} (which causes toxic overloading) is also taken as a disturbance variable.

So, a control strategy should be made which holds good for various values of the disturbances.

Such a control strategy can be realised by performing the relative gain analysis for the system.

Similarly, relative gains were computed for a particular flow rate (Table 5.1) by making a 10% perturbation in each

T A B L E 5.1
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RELATIVE GAIN ARRAY FOR THE 20 CONTROL SETS OBTAINED
AT STEADY STATE 'a' FOR A FLOW RATE OF F=1.0 LITERS/DAY.

		CX0	CS0	CC0
(1)	CC	-14.90452	-109.0395	124.9438
	PC	13.86803	111.0693	-123.9374
	PH	2.036417	-1.02999	-0.06476
		CX0	CS0	CC0
(2)	CS	0.70903	0.289870	0.001090
	CC	-11.8048	-112.1218	124.9278
	PC	12.09580	112.8320	-123.9278
		CX0	CS0	CC0
(3)	CX	1.115840	-0.160200	0.0001800
	CC	18.47280	-142.2297	124.75680
	PC	-18.5886	143.34570	-123.7570
		CX0	CS0	CC0
(4)	CC	11231.064	-11291.992	124.94380
	PC	13.868030	111.069300	-123.9374
	OCH4	71.430209	-70.539901	0.1097102
		CX0	CS0	CC0
(5)	CC	-1.12146	1.343880	0.77758
	OCH4	0.087545	0.696277	0.216178
	PH	2.033922	-1.040158	0.006236
		CX0	CS0	CC0
(6)	CX	0.47677	0.399252	0.123977
	CC	-0.543077	5.175179	-3.532101
	PH	1.166307	-4.57433	4.4081200
		CX0	CS0	CC0
(7)	CS	5.548716	-18.27044	13.72172
	CC	9.351408	85.218750	-93.57015
	PH	-13.90012	-55.94830	80.848430

		CX0	CS0	CC0
(8)	PC	-1.12838	1.352230	0.7761501
	OCH4	0.094661	0.687801	0.2175380
	PH	2.033710	-1.040034	0.0063154
		CX0	CS0	CC0
(9)	CX	0.498269	0.331161	0.120569
	PC	-0.62534	5.032660	-3.40732
	PH	1.127070	-4.41383	4.286750
		CX0	CS0	CC0
(10)	CS	3.409475	-10.25540	7.845934
	PC	5.346540	48.721880	-53.07143
	PH	-7.75604	-37.46940	46.225400
		CX0	CS0	CC0
(11)	CS	0.594170	0.2927301	0.1130900
	OCH4	0.078168	0.7074331	0.2143972
	PH	0.327658	-0.000171	0.6725124
		CX0	CS0	CC0
(12)	CX	1.117674	-0.1400410	0.0223601
	OCH4	-0.11768	0.94050601	0.1771700
	PH	0.000006	0.19953601	0.8004566
		CX0	CS0	CC0
(13)	CX	0.446093	0.42506001	0.1288401
	CS	0.357022	1.18126601	-0.538230
	PH	0.196880	-0.6053302	1.4004401
		CX0	CS0	CC0
(14)	CX	1.117678	-0.1175000	-0.000177
	PC	0.000603	0.21767201	0.7823241
	OCH4	-0.11768	0.89982801	0.2176530
		CX0	CS0	CC0
(15)	CX	0.435050	0.43205001	0.1328900
	CS	0.432591	1.35938000	-0.801970
	PC	0.132360	-0.801437	1.6090770

		CX0	CS0	CC0
(16)	CX	0.439863	0.4290001	0.131127
	CS	0.429521	1.3517660	-0.79129
	CC	0.130605	-0.790776	1.600171
		CX0	CS0	CC0
(17)	CX	1.317690	-0.000119	-0.317570
	CS	-0.00001	0.4924801	0.507525
	QCH4	-0.31708	0.5076330	0.810051
		CX0	CS0	CC0
(18)	CX	1.117678	-0.117502	-0.000175
	CC	0.000004	0.2163050	0.7030901
	QCH4	-0.11768	0.9011960	0.2164850
		CX0	CS0	CC0
(19)	CS	0.608273	0.3927850	-0.001058
	PC	0.215358	-0.000221	0.7840620
	QCH4	0.176368	0.6074351	0.2161952
		CX0	CS0	CC0
(20)	CS	0.608286	0.2927851	-0.001072
	CC	0.216712	-0.000222	0.7835091
	QCH4	0.175000	0.6074370	0.2175625

of the three manipulated variables C_{XO} , C_{SO} and C_{CO} . This yielded $6C_3$ i.e. 20 possible relative gains. The best configuration should be chosen from these twenty possible relative gains.

The following criteria for discarding certain control loop possibilities was used. It can be seen from Table 5.1 certain controlled variables, when they exist together in a relative gain array or a control configuration yielded control loops with high interaction between the loops, as denoted by their relative gain values. They should be discarded.

The following sets of controlled variables, if existing together, were found to give high interacting loops (see Table 5.1).

- (a) C_C , P_C and pH as seen in Set No. 1.
- (b) C_C and P_C as two of the three variables in a set. This occurs in three cases (Set No. 2, 3 and 4)
- (c) C_C and pH as two of the three variables in a set. They occur in three cases (Set No. 5, 6 and 7)
- (d) P_C and pH as two of the three variables in a set. They occur in three cases (Set No. 8, 9 and 10).

Thus from the twenty possible control configuration, 10 are discarded this way. The reason for this high interaction is that C_C is the concentration of dissolved carbon dioxide, P_C is the partial pressure of carbon dioxide and pH, depends on the concentration of carbon dioxide. This close relationship between them make them yield control loops with high interaction.

From the remaining 10 relative gain configurations, the best ones are to be chosen. For this, the best variable among P_C , pH and C_C should be considered, as one of the variables of the relative gain array. These three variables are interrelated and behave in a similar manner. Therefore it is difficult to choose among the three.

pH is considered as the best measurable among them, p_C is also easily measurable and C_C is comparatively difficult to measure. This reduces to three controlled variable sets as seen from Table (5-1) (having pH)

- (i) C_X , QCH_4 and pH, Set No. 12
- (ii) C_S , QCH_4 and pH, Set No. 11
- (iii) C_X , C_S and pH, Set No. 13.

In addition to these three sets, two other sets having P_C , i.e., (C_X, QCH_4, P_C) and (C_X, C_S, P_C) are also considered.

The other remaining five sets have been rejected. The rejection lies either in the set having a variable which is comparatively difficult to measure or in the form of a poor relative gain array, denoting high interactions between the loops.

The relative gain analysis is repeated for different flow rates, each time yielding twenty relative gains^{arrays}. All the configurations got with each of the flow rates were similar in nature. Using the same criteria for discarding control loops, the five control configuration selection was confirmed, for all flow rates.

In order to select the best among these five control configurations, an index is used formulated as

$$\lambda_{\text{L.S.N.I.}} = \sum_{i=1}^3 (\lambda_i^* - 1)^2$$

We called it the least-square non-interaction index where λ_i^* is the best possible relative gain got considering that only one manipulated variable controls one controlled variable.

The smaller the value of least square non-interaction index, the better is the control configuration.

Figure 5.1 is a plot of least square non-interaction index versus flow rate, F . The plot indicates that there is a sharp change in least square non-interaction index for each of the configurations around a value of $F = 1.35$ lit/day. We have already seen that the rate of methane production increases and reaches a maximum value at $F = 1.5$ lit/day (Figure 3.2). To exploit this methane production to the fullest extent, pairs of control configurations are considered where in a configuration is used for a range of F from 0 to 1.35 lit/day and its pair is used for a range of F beyond 1.35 lit/day. The 'configuration pair' which operates with least square non-interaction index would obviously be the best pair of configuration available.

This is easily seen from Figures 5.2 and 5.3. Three sets are considered.

- (1) Split range control: Configuration $C_X - C_{X_0}/QCH_4 - C_{S_0}/pH - C_{C_0}$ used for a range of F from 0-1.35 lit/day,

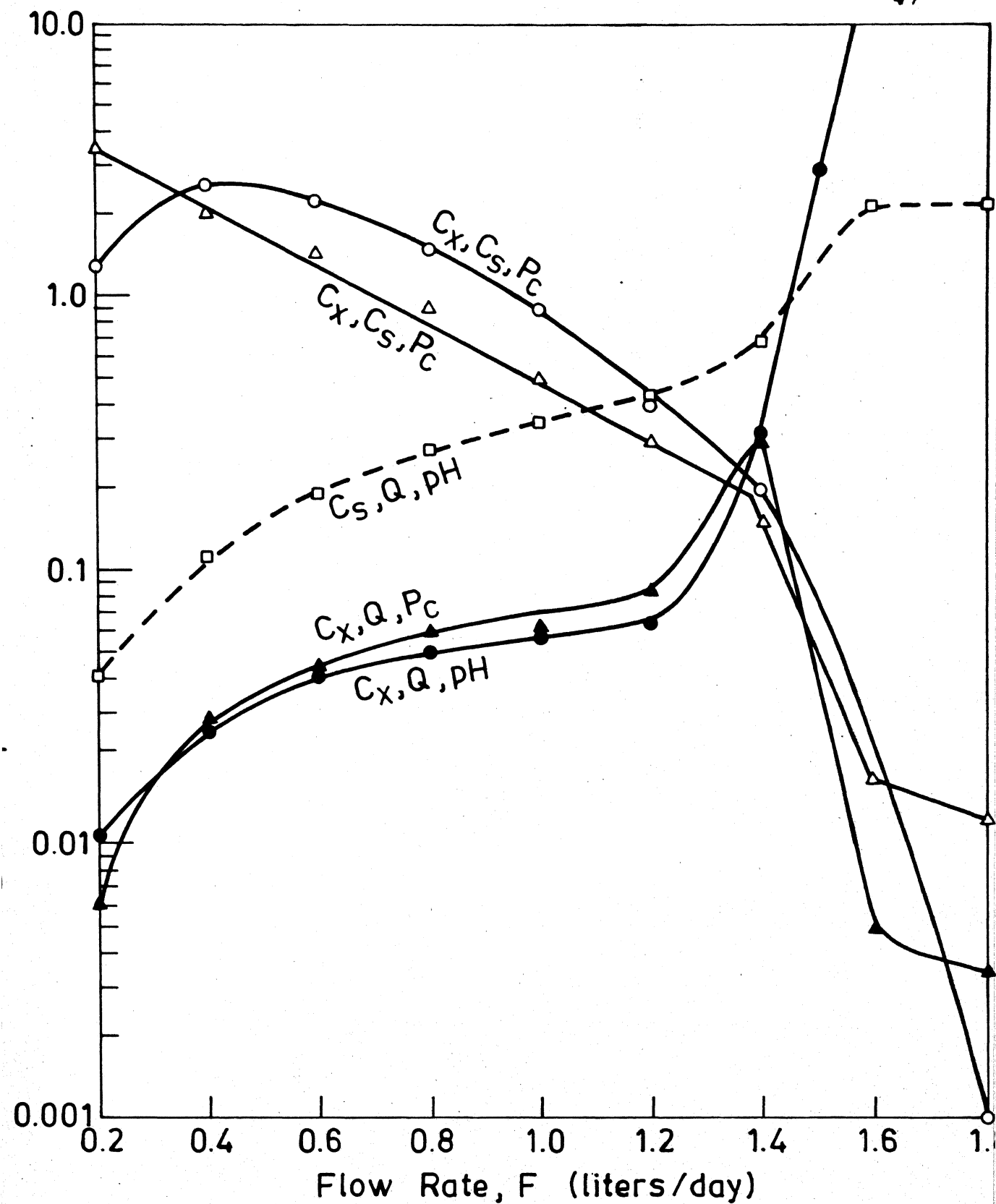


Fig. 5.1. Plot of Least Square Non Interaction Index of Control Configurations for Different Flow Rates.

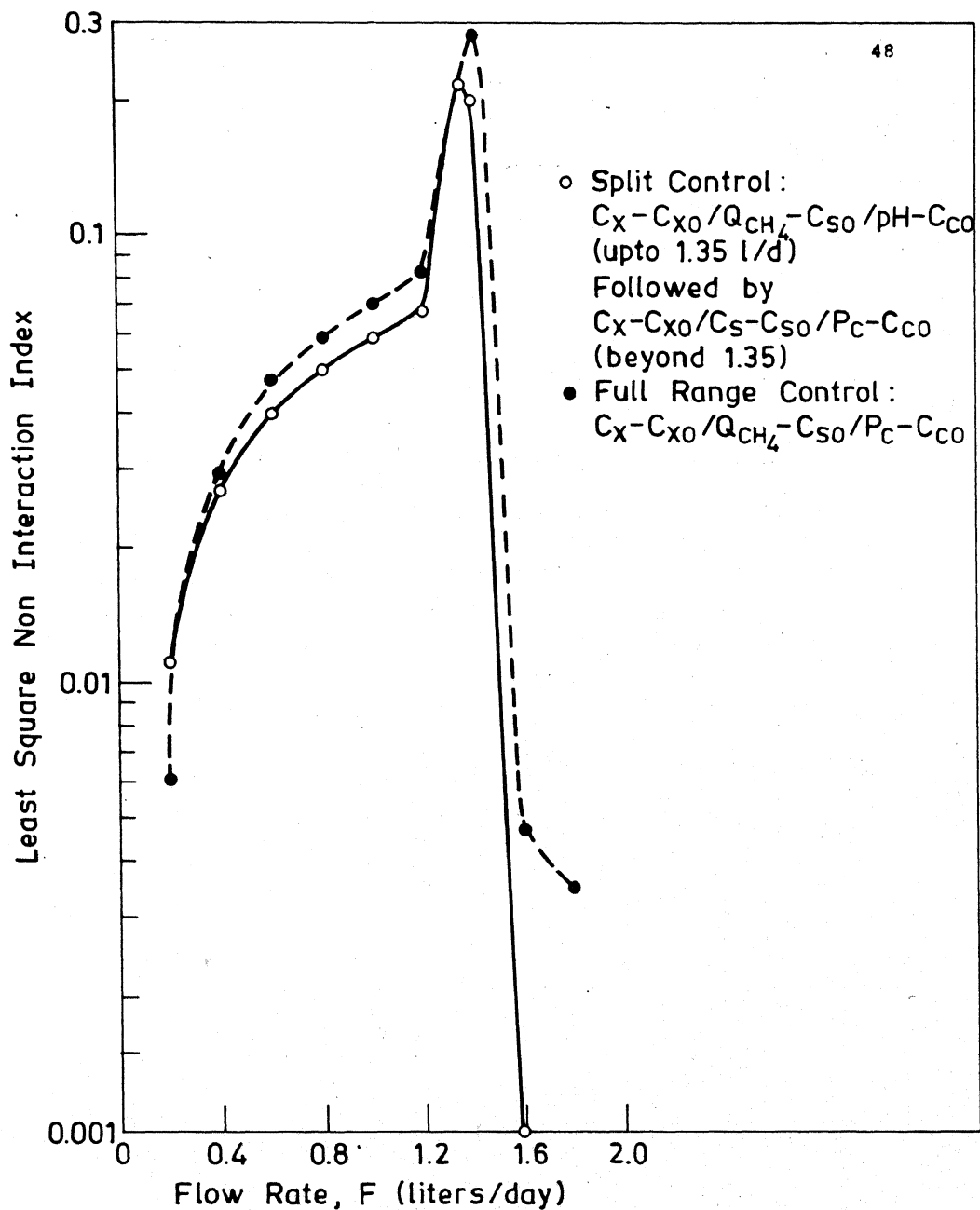


Fig. 5.2. Plot of Least Square Non Interaction Index vs Flow Rate, F.

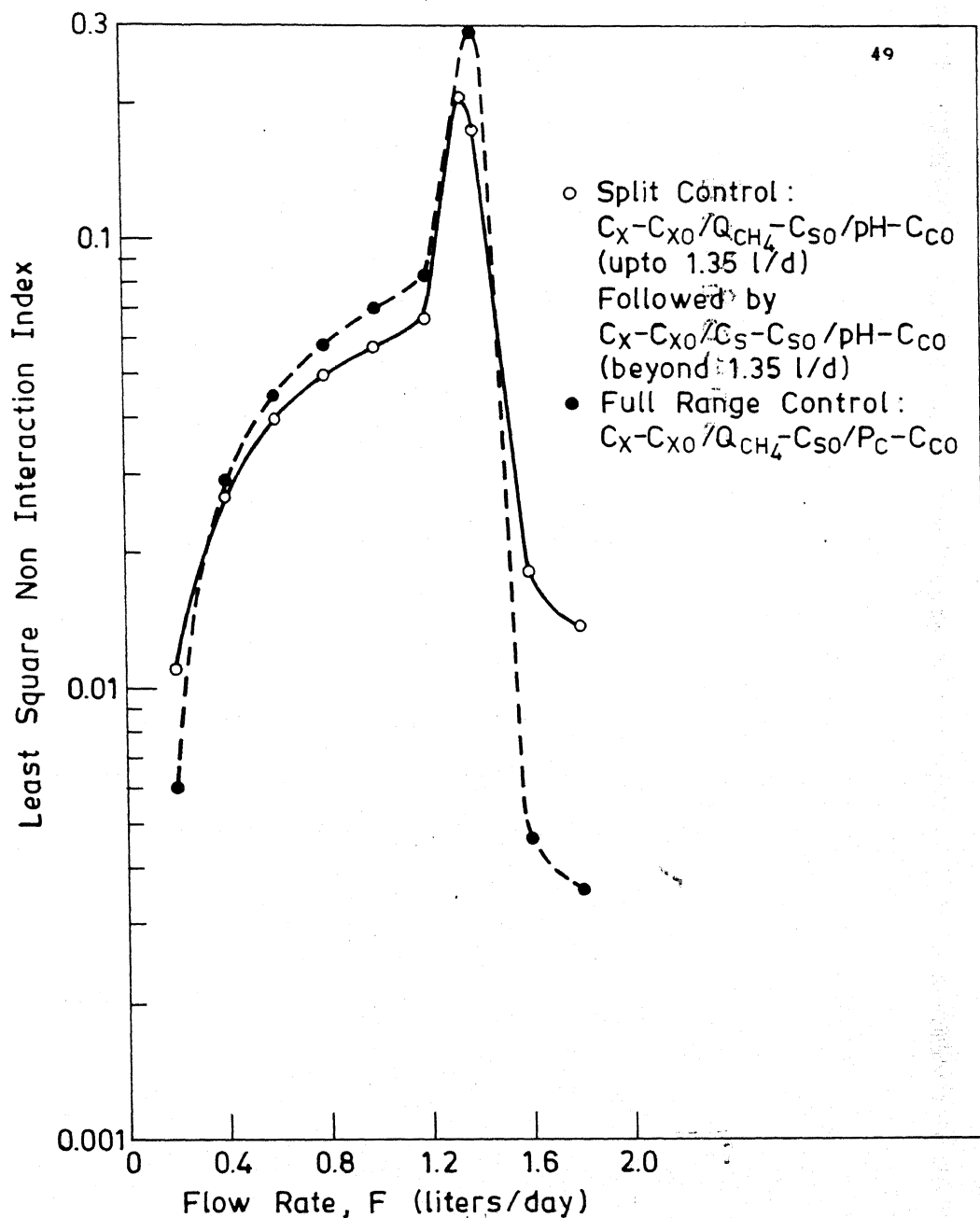


Fig. 5.3. Plot of Least Square Non Interaction Index vs Flow Rate, F.

sequenced by configuration $C_X - C_{X_0}/C_S - C_{S_0}/P_C - C_{C_0}$ operating for a range of F beyond 1.35 lit/day.

(2) Split range control: Configuration $C_X - C_{X_0}/QCH_4 - C_{S_0}/pH - C_{C_0}$ operating for a range of F from 0 to 1.35 lit/day sequenced by configuration $C_X - C_{X_0}/C_S - C_{S_0}/pH - C_{C_0}$ operating for a range of F beyond 1.35 lit/day.

(3) Full range control: We have a single configuration $C_X - C_{X_0}/QCH_4 - C_{S_0}/P_C - C_{C_0}$ operating in the full range of F (0 to 2 lit/day).

The Figures 5.2 and 5.3 indicate that all the three sets can be employed with equal benefit in controlling the anaerobic digestion process.

However, controlled variable set $C_X - QCH_4 - P_C$ seems to provide the best control since it is operable in the whole range of F and it also eliminates the difficulty of changing two controlled variables (other than C_X) beyond a particular range of the flow rate.

5.2.2 Toxic Loading

The relative gain analysis was performed for different values of the second disturbance variable, C_{T_0} . As before, the five control configurations were confirmed and compared using the least square non-interaction index (Table 5.2).

Figure 5.4 indicates that the toxicity has virtually no effect on the configurations.

Table 5.2

Least Square Non-Interaction Index of the Five Configurations for Different Toxicities and Flow Rates

Flow rate F (l/d)	Toxicity, $C_{T_O} \times 10^{-6}$ (m/s)			
	0	1	2	3
$C_X - C_{X_O}/C_S - C_{S_O}/P_C - C_{C_O}$				
0.6	2.39183	2.36981	2.34624	2.32210
0.8	1.52991	1.49780	1.47097	1.44274
1.0	0.90327	0.88497	0.86706	0.84933
1.2	0.48337	0.47319	0.46325	0.45362
$C_S - C_{X_O}/QCH_4 - C_{S_O}/pH - C_{C_O}$				
0.6	0.19389	0.19644	0.19912	0.20103
0.8	0.27320	0.27590	0.27864	0.29843
1.0	0.35751	0.36055	0.36363	0.36677
1.2	0.45691	0.46097	0.46513	0.46943
$C_X - C_{X_O}/QCH_4 - C_{S_O}/pH - C_{C_O}$				
0.6	0.04015	0.04067	0.04411	0.04160
0.8	0.05002	0.05057	0.05102	0.05196
1.0	0.05720	0.05774	0.05836	0.05903
1.2	0.06677	0.06821	0.06982	0.07161
$C_X - C_{X_O}/C_S - C_{S_O}/pH - C_{C_O}$				
0.6	1.44082	1.42961	1.40638	1.38262
0.8	0.90524	0.88850	0.87217	0.74528
1.0	0.50731	0.49965	0.49240	0.48389
1.2	0.30279	0.30390	0.30412	0.30426
$C_X - C_{X_O}/QCH_4 - C_{S_O}/P_C - C_{C_O}$				
0.6	0.04550	0.04613	0.04684	0.04771
0.8	0.05390	0.05989	0.06049	0.06607
1.0	0.06123	0.07187	0.07255	0.07326
1.2	0.09128	0.08147	0.08671	0.08812

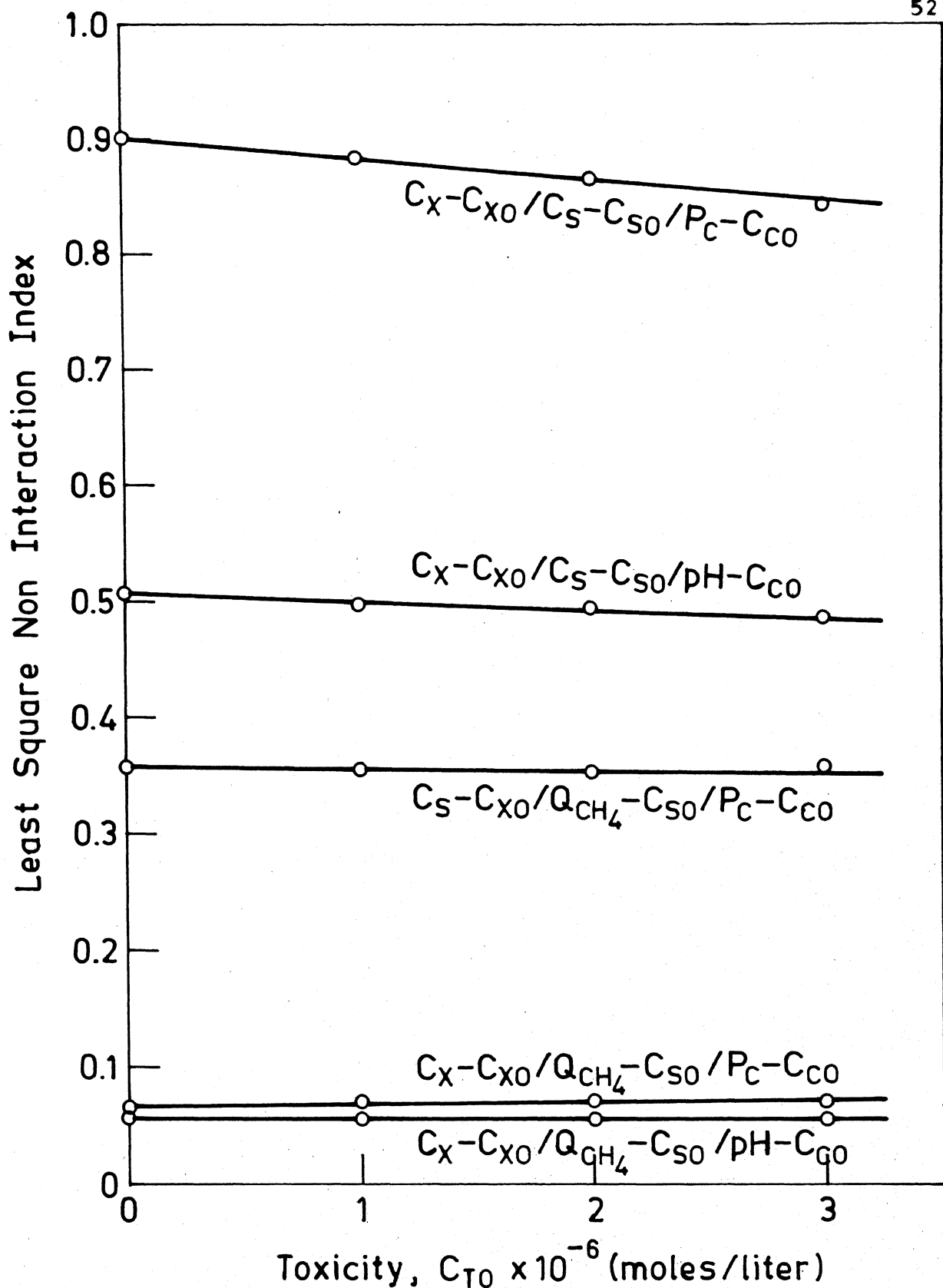


Fig. 5.4. Plot of Least Square Non Interaction Index vs Toxicity, C_{T0} at a Flow Rate, $F = 1.0$ liters/day.

5.3 Dynamic Analysis

The dynamic relative gain analysis was performed using the dynamic model of the digester. This was done by simulating the response of the controlled variable to the change in manipulations and then computing the dynamic relative gain by using the modified form of Witcher and McAvoy method, described earlier.

Figures 5.5 to 5.9 represents the dynamic responses of the six controlled variables to the change in the manipulated variables.

Table 5.3 compares the least square non-interaction index of the five control configurations for both the steady state and dynamic analysis. It can be seen that the least square non-interaction dynamic index is a shade better than the least square non-interaction static index. Also, it confirms that the $C_X - C_{X_0} / QCH_4 - C_{S_0} / pH - C_{C_0}$, $C_X - C_{X_0} / QCH_4 - C_{S_0} / P_C - C_{C_0}$ configurations are the best possible for an anaerobic digester.

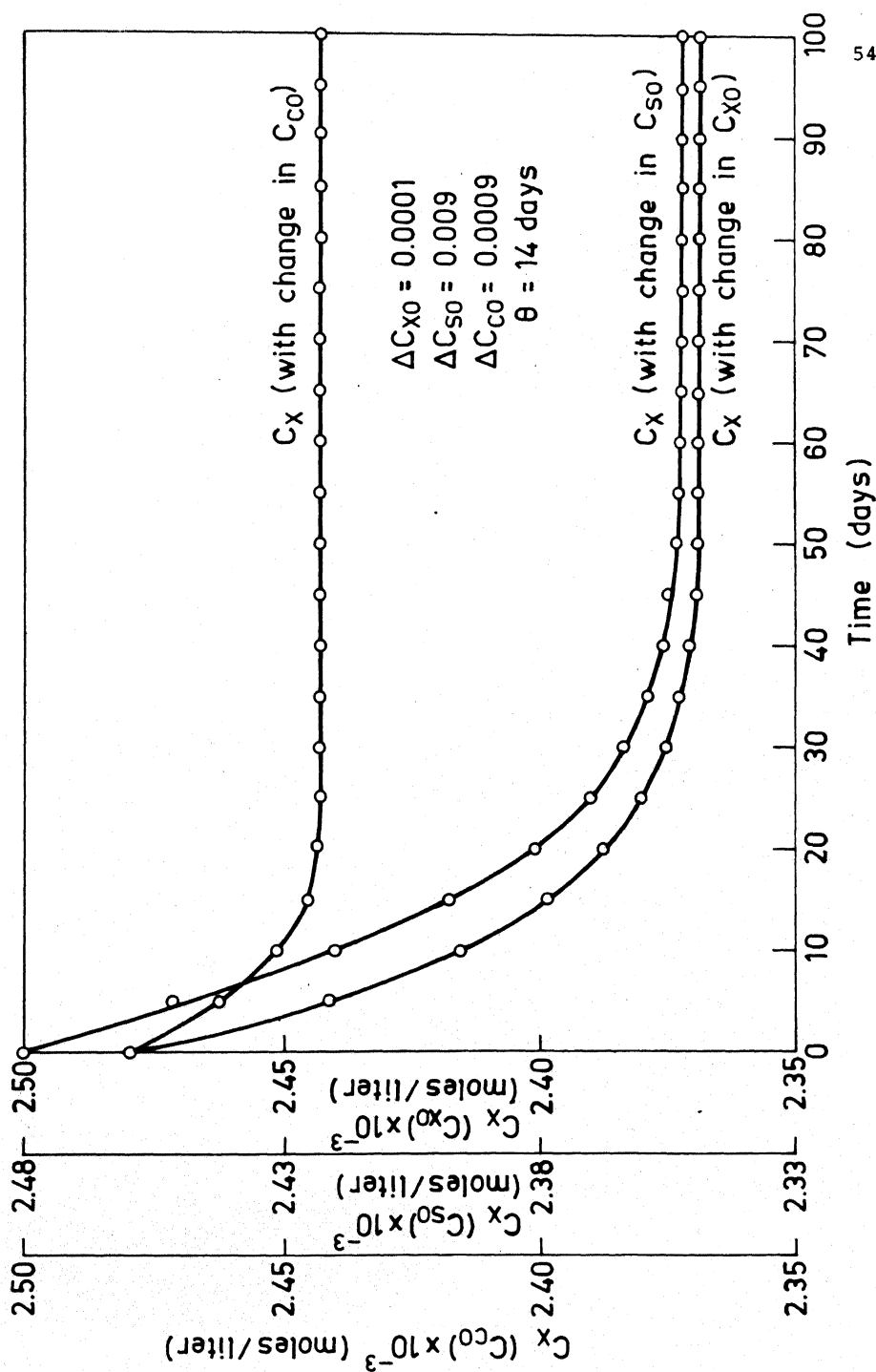


Fig. 5.5. Dynamic Response of Micro Organism Concentration to the Change in Manipulated Variables.

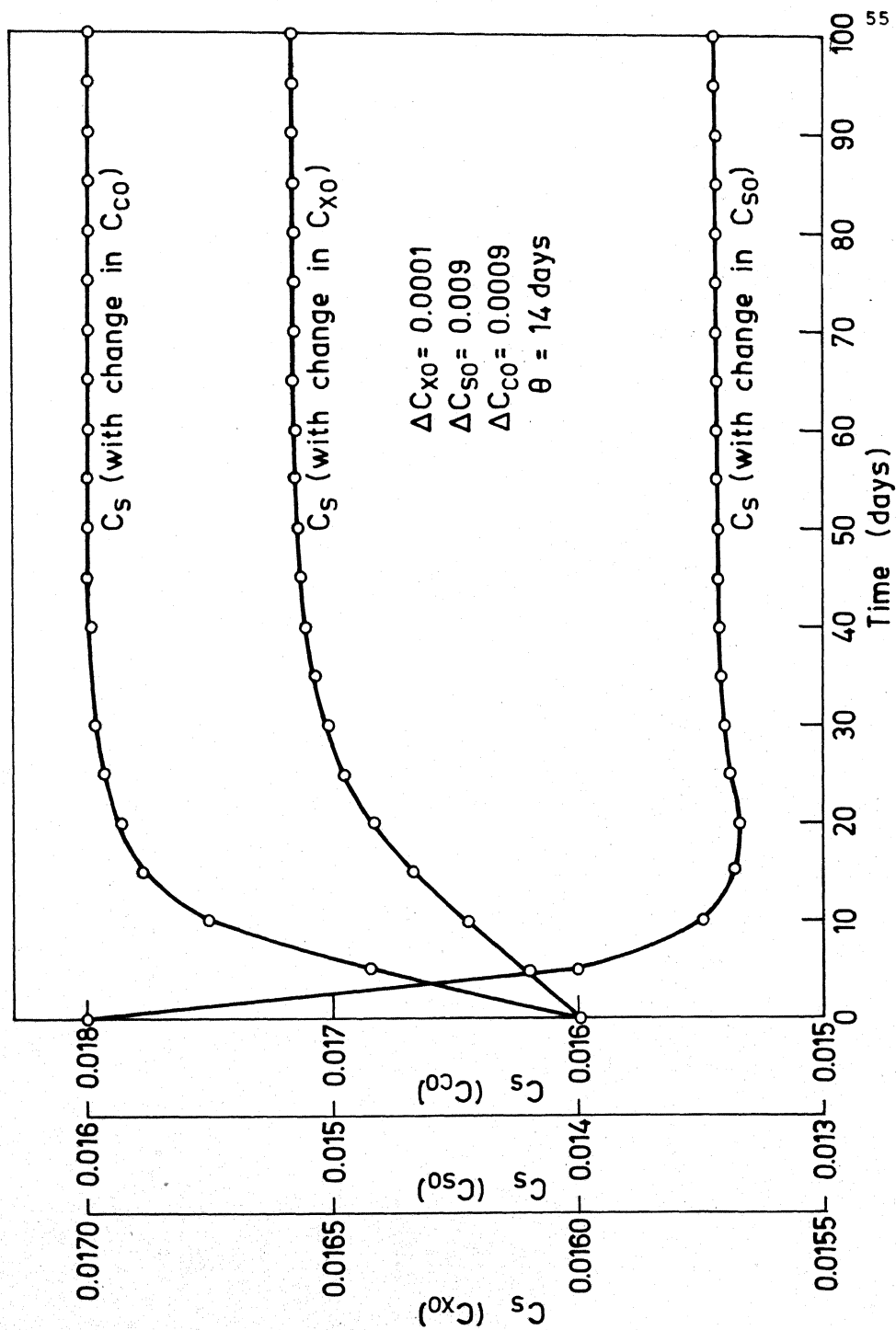


Fig. 5.6. Dynamic Response of Substrate Concentration to the Change in Manipulated Variables.

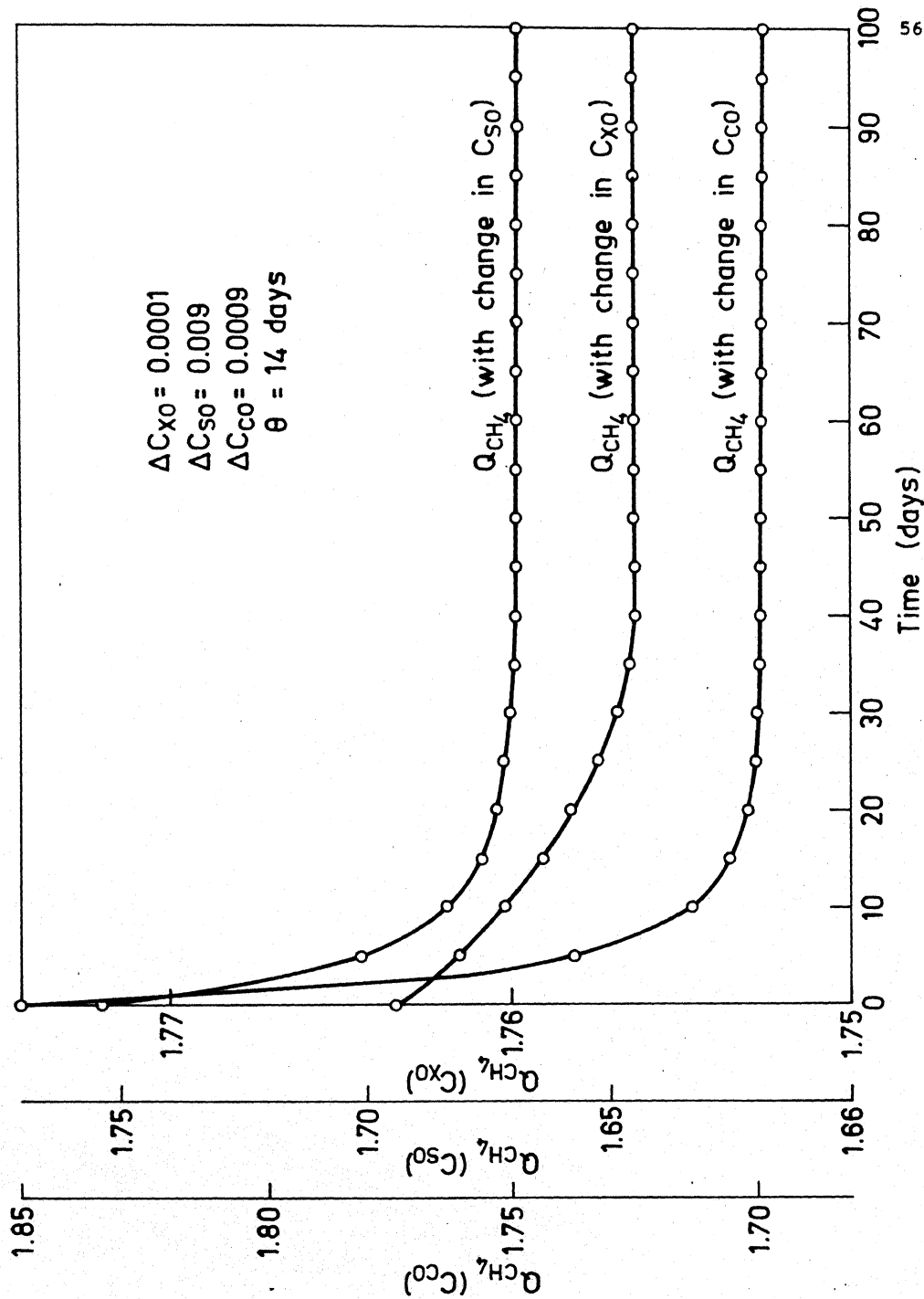


Fig. 5.7. Dynamic Response of Methane Production Rate to the Change in Manipulated Variables.

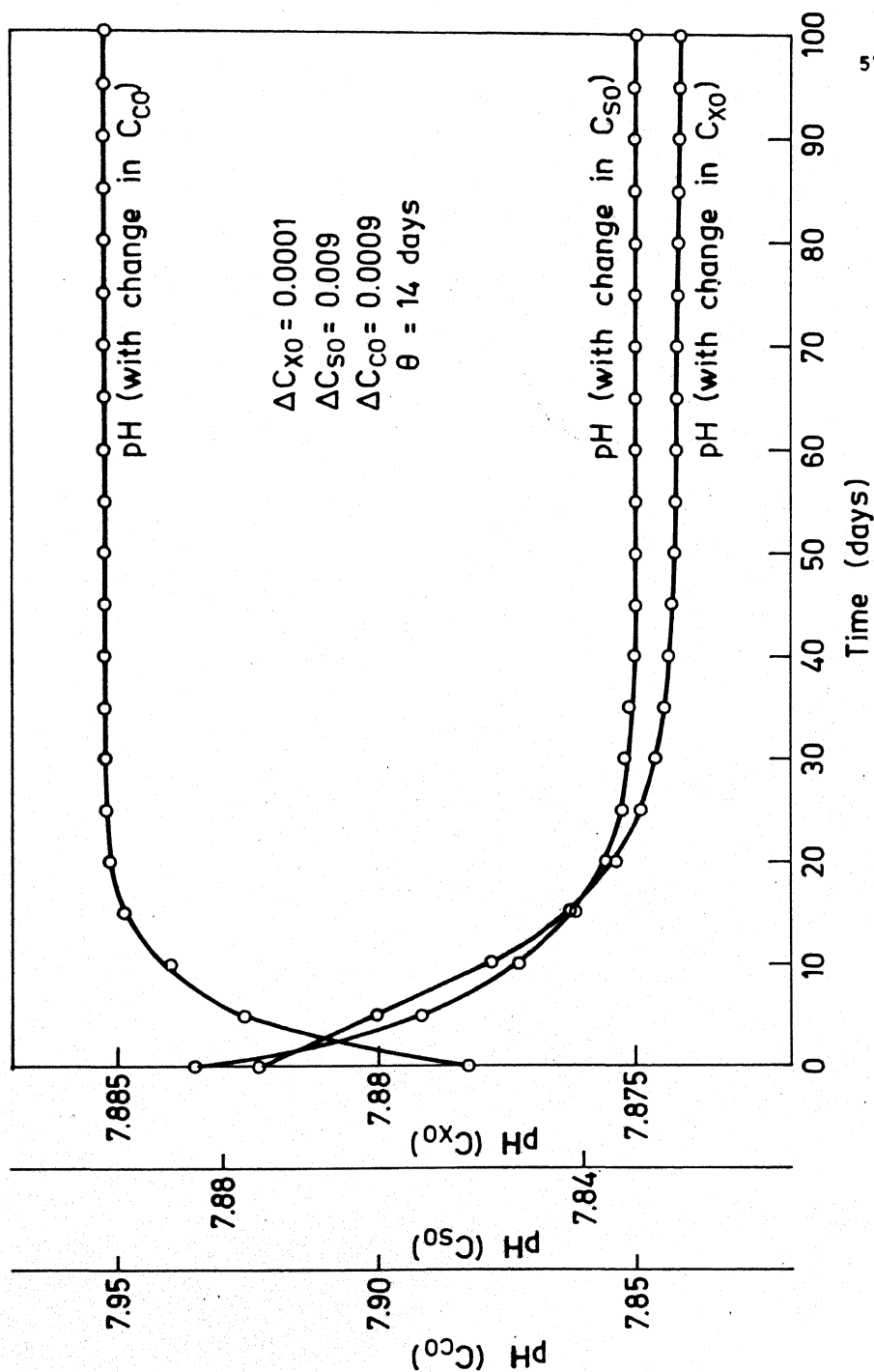


Fig. 5.8. Dynamic Response of pH to the Change in Manipulated Variables.

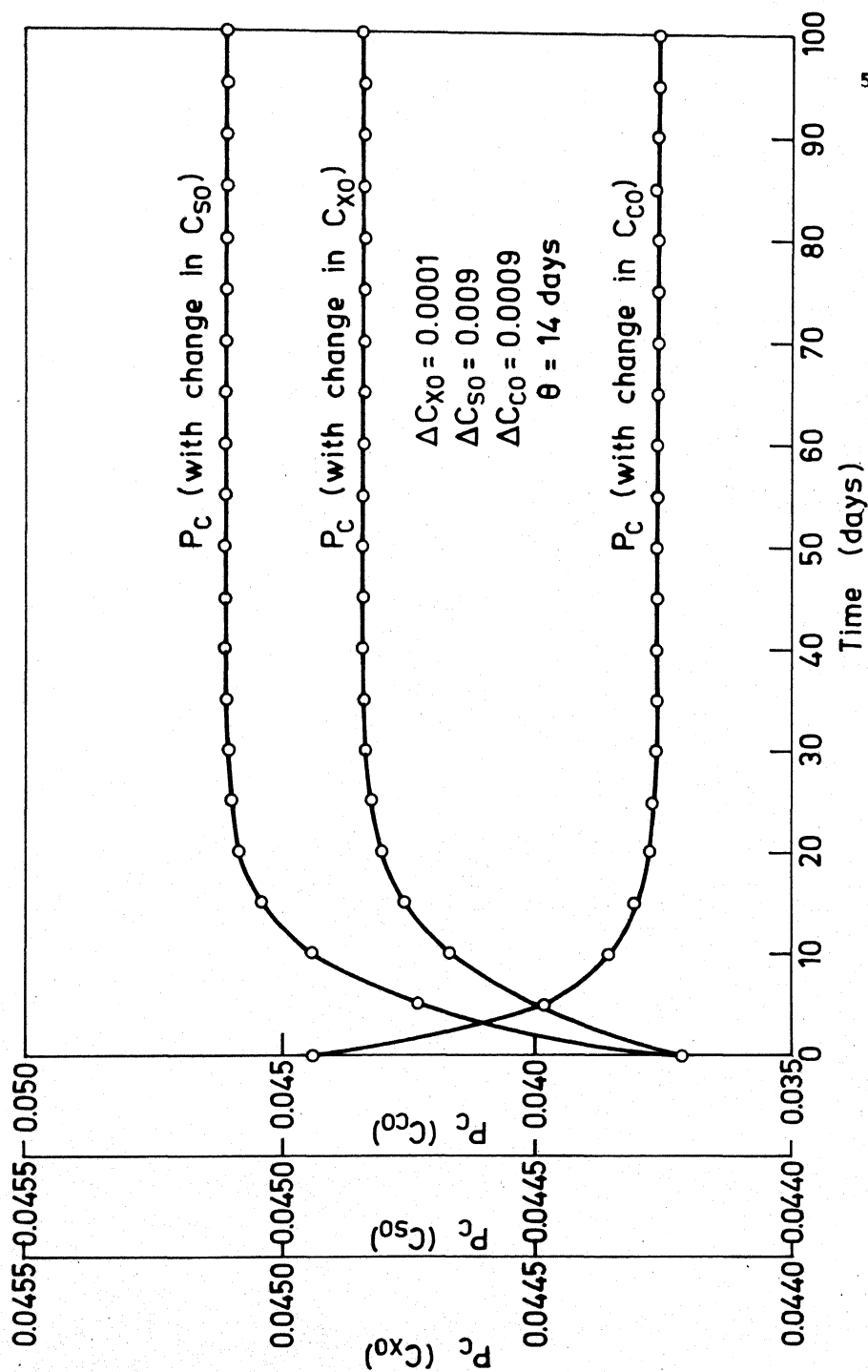


Fig. 5.9. Dynamic Response of Partial Pressure of Carbon di Oxide to the Change in Manipulated Variables.

Table 5.3

Comparison of Least Square Non-Interaction Index for the Control Configurations in Steady State and Dynamic Analysis

Control configuration	Least square non-interaction index in steady state analysis	Least square non-interaction index in dynamic analysis
	at $F = 1.0 \text{ lb/hr}$	at $F = 1.0 \text{ lb/hr}$
$C_S - C_{XO}/QCH_4 - C_{SO}/pH - C_{CO}$	0.35751	0.26048
$C_X - C_{XO}/QCH_4 - C_{SO}/pH - C_{CO}$	0.05720	0.02925
$C_X - C_{XO}/C_S - C_{SO}/PH - C_{CO}$	0.50731	0.33127
$C_X - C_{XO}/C_S - C_{SO}/P_C - C_{CO}$	0.90327	0.56231
$C_X - C_{XO}/QCH_4 - C_{SO}/P_C - C_{CO}$	0.06123	0.03085

Chapter 7

CONCLUSION

System engineering tools like the steady state and dynamic relative gains succeed in their attempt in quantifying the process operation and developing a more rational control strategy for the anaerobic digestion process.

The results of the relative gain analysis bring out the following facts:

(1) The present day control practice is confirmed:

(a) The present day operation is in controlling the pH by scrubbing of carbon dioxide and recycling it back to the digester. Relative gain analysis gives a configuration $C_X - C_{X_0}/QCH_4 - C_{S_0}/pH - C_{C_0}$ in which pH is controlled by manipulating the inlet carbon dioxide concentration.

(b) Another recent practice is in controlling the rate of methane production by recycling the concentrated sludge. The relative gain analysis suggests that the rate of methane production is to be controlled by manipulating the inlet substrate concentration, which can be done by recycling the concentrated sludge.

(2) New controlled possibilities are suggested:

The present day practice of controlling pH by scrubbing and recycling of carbon dioxide does not hold good in situations where hydraulic loadings exceed a particular value. A new controlled possibility $C_X - C_{X_0}/QCH_4 - C_{S_0}/P_C - C_{C_0}$ wherein the partial pressure of carbon dioxide

is controlled by manipulating the inlet carbon dioxide concentrations holds good both for hydraulic and toxic loadings.

The same benefit can also be achieved by having split control:

(a) Configuration $C_X - C_{X_0}/QCH_4 - C_{S_0}/pH - C_{C_0}$ operating upto a hydraulic load of 1.35 lit/day sequenced by configuration $C_X - C_{X_0}/C_S - C_{S_0}/pH - C_{C_0}$ operating at hydraulic loads beyond 1.35 lit/day. It should be noted that is a change in the controlled variable from QCH_4 to C_S during the sequential operation.

(b) Configuration $C_X - C_{X_0}/QCH_4 - C_{S_0}/pH - C_{C_0}$ operating upto a hydraulic load of 1.35 lit/day sequenced by configuration $C_X - C_{X_0}/C_S - C_{S_0}/P_C - C_{C_0}$ operating beyond 1.35 lit/day. Here, it should be noted that two controlled variables change (QCH_4 to C_S and pH to P_C) during the sequential change.

Chapter 7

SUGGESTIONS FOR FUTURE WORK

The following are the suggestions for future work:

- (1) The process parameters like K_s , K_i , K_{La} , K_a , S_{M_X} , S_{C_X} and S_{X_S} should be identified. There exists an uncertainty in the substrate composition and the associated parameters and in order to have faith in the control parameters, these process parameters need to be identified by employing the input-output data of the process.
- (2) The relative gain analysis of the anaerobic digestion process aids the multivariable control pairing decision, however, other control strategies like the adaptive control and feed forward control can also be tried for the anaerobic digestion process.
- (3) The relative gain analysis has been done for the continuous feeding of the digester (represented as a CSTR). The analysis also needs to be done for batch feeding and periodic feeding of the digester.
- (4) The current model of the digester considers acetic acid as the lone substrate. Recent research²² indicates that other higher fatty acids can also produce more methane gas by providing the proper biological environment. So focus should be done on modelling and simulation using different substrates, individually. Not much data is available in the literature and this could be a great help for the operation of the digester. As a corollary,

modelling and simulation should also be done for different substrates coexisting together.

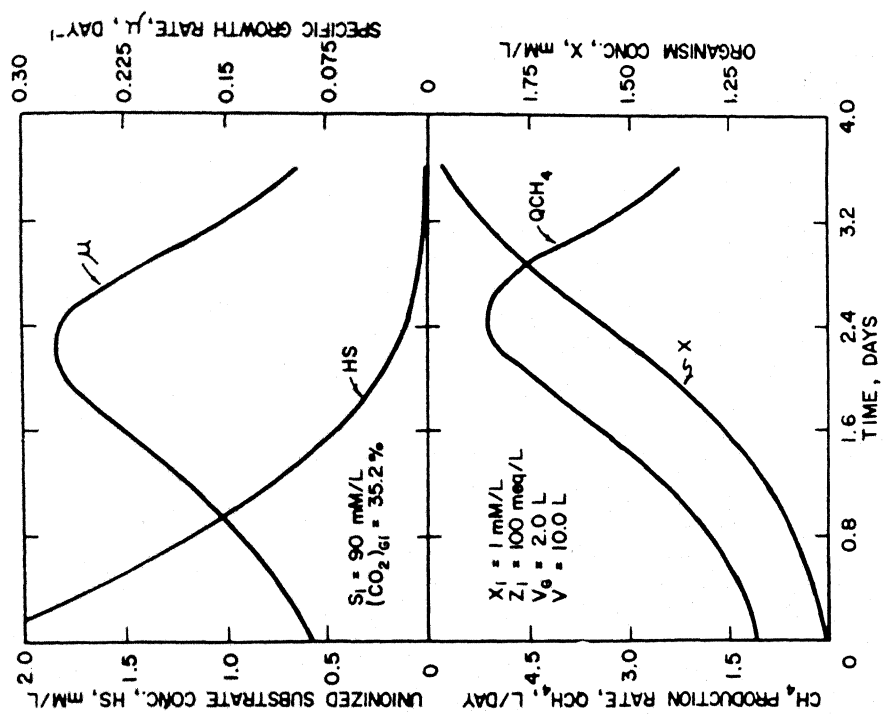
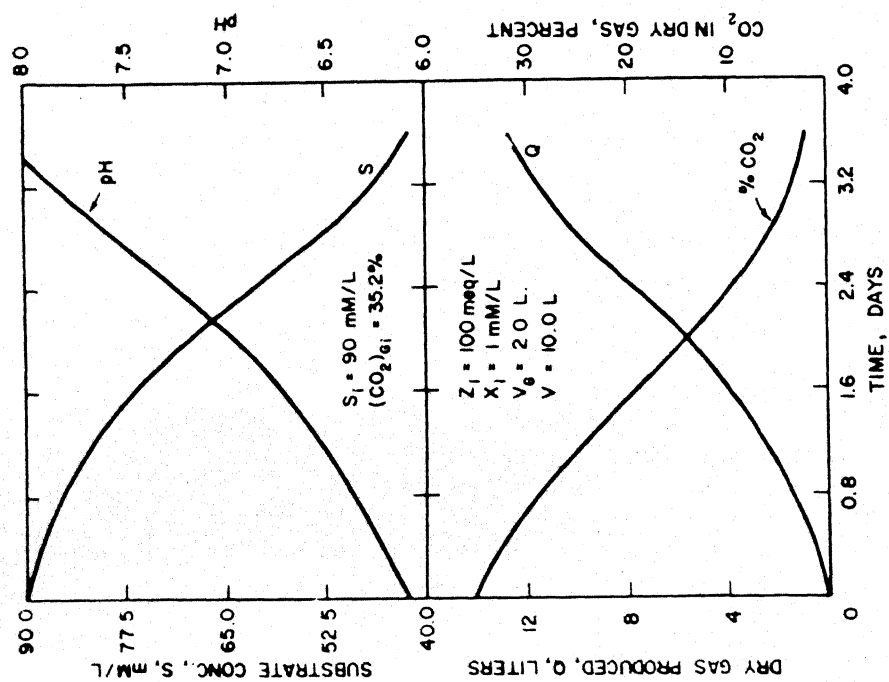
- (5) Membrane separation process like dialysis can separate the two phases — the acetogenic phase and the methanogenic phase, co-existing in a digester. If model is available for both of these phases, a combined control strategy for both of these phases can be developed. The model for the methanogenic phase is currently in use since it is considered as the rate limiting step of the digestion process. Our focus should be on modelling the acetogenic phase.

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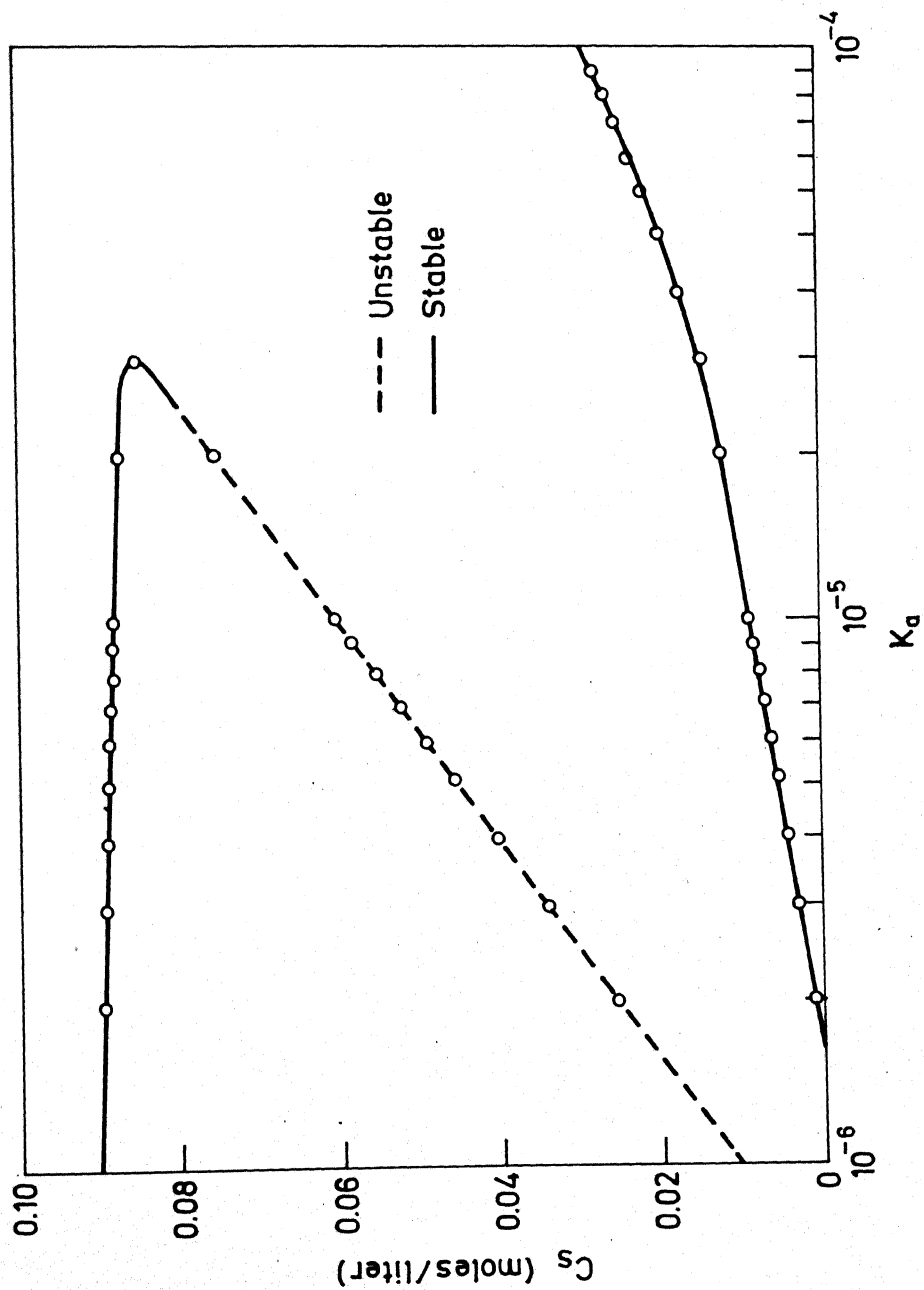
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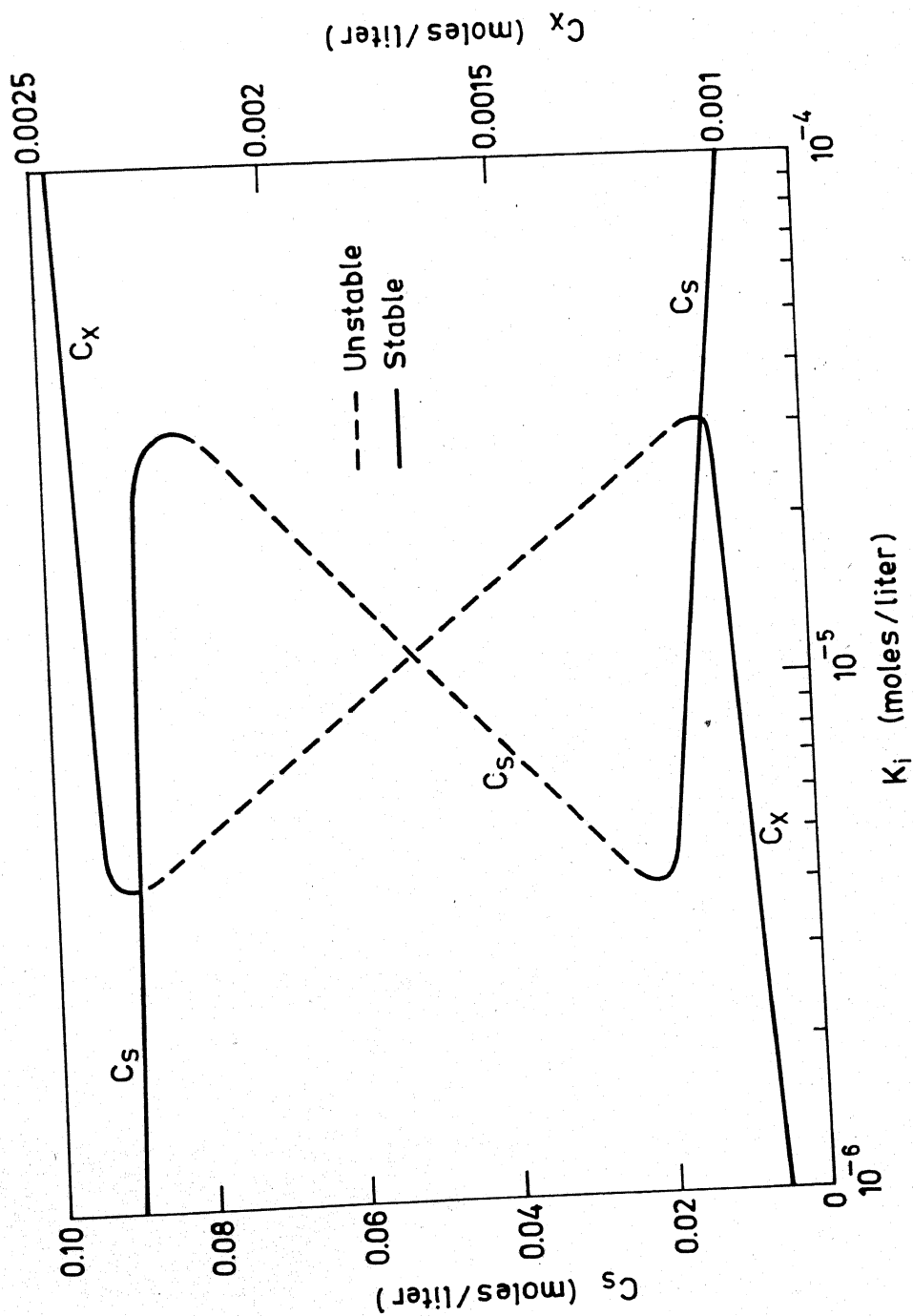
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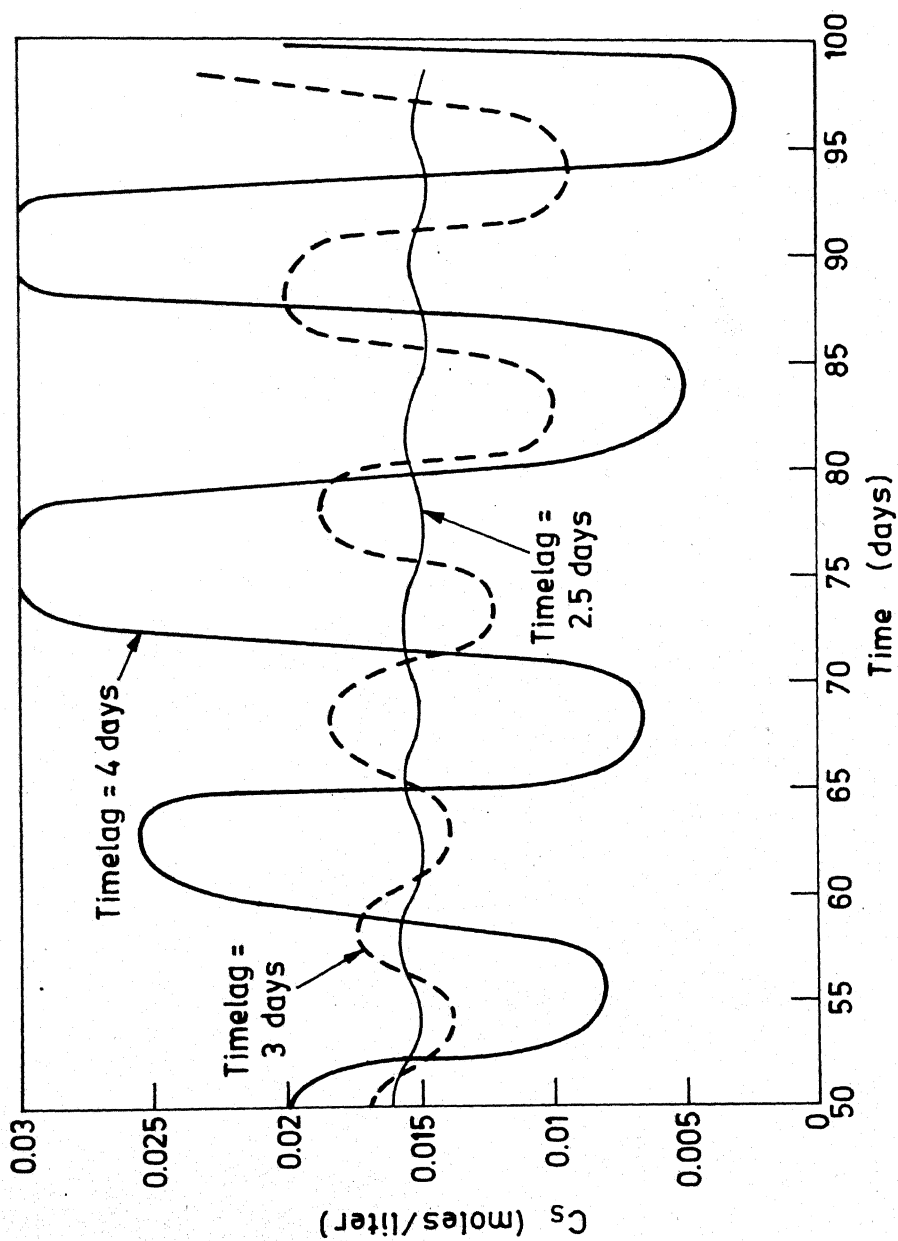
Appendix A.1. Batch Reactor Simulation Results of Andrews and Graef.



Appendix A.2. Dependence of Stationary Values of Substrate Concentration on K_a . $K_{La} = 30$, $K_i = 0.3 \times 10^{-4}$, Other Parameters as in Table 3.2.



Appendix A.3. Dependence of the Stationary Values on K_i . $K_{La} = 30$, Other Parameters as in Table 3.2.



Appendix A.4. Dynamic Behaviour of the System with Timelag. $K_{La} = 30$,
Other Parameters as in Table 3.2.

APPENDIX B.1 =====

PROGRAM FOR GETTING STATIONARY SOLUTIONS ----- BY SOLVING NON-LINEAR EQUATIONS -----

THE PARAMETERS USED ARE

FC=FLOW RATE, L/DAY.
AK=HENRY'S LAW CONSTANT, MOL/L. ATM.
AKA=ACID DISSOCIATION CONSTANT, MOL/L.
AKI=INHIBITION CONSTANT, MOL/L.
AKLA=OVERALL GAS TRANSFER FILM COEFF, /DAY.
AK1=IONISATION CONSTANT OF BICARBONATE, MOL/L.
AKS=SATURATION CONSTANT, MOL/L.
SXS=ORGANISM YIELD.
SCX=CO₂ YIELD.
SMX=CH₄ YIELD.
V=DIGESTER LIQUID VOLUME, L.
VG=VOLUME OF GAS SPACE, L.
HMU=MAX. SPECIFIC GROWTH RATE, /DAY.
AKT=TOXICITY INFLUENCE RATE, /DAY.
SP=CONVERSION FACTOR, L/MOL.
P=TOTAL PRESSURE, ATM.
CX0, CS0, CCO, CZ0, CTO=INLET CONCENTRATIONS OF ORGANISMS, LIMITING
SUBSTRATE, DISSOLVED CO₂, NET CATION AND TOXIC COMPONENTS RESPECTIV

DIMENSION X(30)

1 COMMON FO, AK, AKA, AKI, AKLA, AK1, AKS, SXS, SCX, SMX, V, VG, HMU, AKT, SP,
1 P, CX0, CS0, CCO, CZ0, CTO
1 DATA FO, AK, AKA, AKI, AKLA, AK1, AKS, SXS, SCX, SMX, V, VG, HMU, AKT, SP, P,
1 CX0, CS0, CCO, CZ0, CTO/0.6, 0.024593, 0.316E-4, 1.0E-3, 30.0, 0.1E-5,
1 0.333E-4, 0.02, 47.0, 47.0, 10.0, 2.0, 0.4, 2.0, 25.5, 0.93421, 0.001,
1 0.09, 0.0081, 0.1, 1.0E-5/
OPEN(UNIT=31, DEVICE='DISK')

X(1)=0.0025

X(2)=0.010

X(3)=0.001

X(4)=0.039

TYPE*, (X(1), I=1, 5)

N=4; NUMSIG=6; MAXIT=25; IPRINT=1; EPS=1.E-6; ND=31

CALL NONLIN(N, NUMSIG, MAXIT, IPRINT, X, EPS, ASIER, ND)

STOP

END

SUBROUTINE NONLIN(N, NUMSIG, MAXIT, IPRINT, X, EPS, ASIER, ND)

This subroutine solves a system of N simultaneous nonlinear equations. The method used is at least quadratically convergent and requires only $(N^2/2 + 3*N/2)$ function evaluations per iterative step as compared with $(N^2 + N)$ evaluations for NEWTON'S method. This results in a savings of computational effort for sufficient complicated functions. The method does not require the user to furnish any derivatives.

INPUT PARAMETERS FOLLOW :

N = Number equations (= number of unknowns)
NUMSIG = Number of significant digits desired.
MAXIT = Maximum number of iterations to be used.

IPRINT = Output option, output if =1; however, failure indications are always output; MAXIT exceeds and singular Jacobian.
 X = Vector of initial guesses.
 EPS = Convergence criterion. Iteration will be terminated if $ABS(F(I)) \cdot LI \cdot EPS, I=1, \dots, N$, where $F(I)$ denotes the I th function in the system.

Convergence criterion is considered to be met if either the number of significant digits requested is achieved or the EPS criterion of the function values is satisfied. To force the iteration to be terminated by one of the criteria, simply set the other one to be very stringent.

OUTPUT PARAMETERS FOLLOW :

NIT = Number of iterations used.
 X = Solution of the system (or best approximation thereof).

REAL X(30), PART(30), TEMP(30), COE(30,31), RELCON, F, FACTOR,
 IHOLD, H, FPLUS, DERMAT, TEST
 DIMENSION ISUB(30), LOOKUP(30,30)
 COMMON/VAR/XR, XQ, XS, XT

DELTA WILL BE A FUNCTION OF THE MACHINE AND THE PRECISION. USE

```

TYPE*, (X(I), I=1,5)
DELTA = 1.E-7
RELCON = 10.E+0**(-NUMSIG)
JTEST = 1
DO 700 M=1, MAXIT
  IQUIT = 0
  FMAX = 0.
  M1 = M-1
  IF (IPRINT.NE.1) GO TO 9
  OPEN(UNIT=ND, DEVICE='DISK')
  WRITE(ND,49) M1, (X(I), I=1,N)
  FORMAT(15,7E18.8/(E23.8,6E18.8))
  TYPE 102, M1, (X(I), I=1,N)
  FORMAT(15,7E18.8/(E23.8,6E18.8))
  DO 10 J=1,N
    LOOKUP(1,J)=J
  
```

The array LOOKUP permits a partial effect without having to interchange rows or columns.

```

DO 500 K=1,N
  IF(K-1) 134,134,131
  KMIN = K-1
  CALL BACK(KMIN,N,X,ISUB,COE,LOOKUP)
  
```

Set up partial derivatives of Kth function..

```

134 CALL AUXFCN(X,F,K)
  FMAX= AMAX1(FMAX,ABS(F))
  IF(ABS(F) .GE. EPS) GO TO 1345
  IQUIT=IQUIT+1
  IF(IQUIT.NE.N) GO TO 1345
  GO TO 725
1345 FACTOR = .001E+00
135 ITALLY = 0.
  
```

```

DO 200 I=K,N
ITEMP = LOOKUP(K,1)
HOLD = X(ITEMP)
PREC = 5.E-6
PREC IS THE FUNCTION OF THE MACHINE SIGNIFICANCE, SIG, AND SHOULD
BE COMPUTED AS PREC = 5.*(-SIG+2). IN THIS INSTANCE WE WERE DEAL-
LING WITH AN 8 DIGIT MACHINE.
ETA = FACTOR*ABS(HOLD)
H = AMIN1(FMAX,ETA)
IF(H.LT.PREC) H=PREC
X(ITEMP) = HOLD+H
IF(K-1) 161,161,151
151 CALL BACK(KMIN,N,X,ISUB,COE,LOOKUP)
161 CALL AUXFCN(X,FPLUS,K)
PART(ITEMP) = (FPLUS-F)/H
X(ITEMP) = HOLD
IF(ABS(PART(ITEMP)).LT.DELTA) GOTO 190
IF(ABS(F/PART(ITEMP)).LE.1.E+15) GOTO 200
190 ITALLY = ITALLY+1
200 CONTINUE
IF(ITALLY.LE.N-K) GOTO 202
FACTOR = FACTOR*10.0E+00
IF(FACTOR.GT.11) GOTO 775
GOTO 135
202 IF(K.LT.V) GOTO 203
IF(ABS(PART(ITEMP)).LT.DELTA) GOTO 775
COE(K,N+1)=0.0E+00
KMAX = ITEMP
GOTO 500

```

Find partial derivatives of largest absolute value.

```

203 KMAX = LOOKUP(K,K)
DERMAX = ABS(PART(KMAX))
KPLUS = K+1
DO 210 I=KPLUS,N
JSUB = LOOKUP(K,I)
TEST = ABS(PART(JSUB))
IF(TEST.LT.DERMAX) GOTO 209
DERMAX = TEST
LOOKUP(KPLUS,1)=KMAX
KMAX = JSUB
GO TO 210
209 LOOKUP(KPLUS,1)=JSUB
210 CONTINUE
205 IF(ABS(PART(KMAX)).EQ.0.0) GOTO 775

```

Set up coefficients for Kth row of triangular linear system to back-solve for the first K values of X(I)

```

ISUB(K) = KMAX
COE(K,N+1)=0.0E+00
DO 220 J = KPLUS,N
JSUB = LOOKUP(KPLUS,J)
COE(K,JSUB)=-PART(JSUB)/PART(KMAX)
COE(K,N+1)=COE(K,N+1)+PART(JSUB)*X(JSUB)
220 CONTINUE
500 COE(K,N+1)=(COE(K,N+1)-F)/PART(KMAX)+X(KMAX)
Back substitute to obtain next approximation to X.
X(KMAX) = COE(N,N+1)

```

```

IF(N.EQ.1) GOTO 610
CALL BACK(N-1,N,X,ISJB,COE,LOOKUP)
IF(M-1) 650,650,625

```

C Test for convergence.

```

625 DO 630 I=1,N
IF(ABS(TEMP(I)-X(I)).GT.ABS(X(I))*RELCON) GOTO 649
630 CONTINUE
JTEST = JTEST + 1
IF(JTEST-3) 650,725,725
649 JTEST = 1
650 DO 660 I = 1,N
660 TEMP(I) = X(I)
700 CONTINUE

```

C OPEN(UNIT=ND,DEVICE='DSK')

WRITE(ND,1753)

1753 FORMAT(5X,'NO CONVERGENCE.MAXIMUM NUMBER OF ITERATIONS USED.')

ASTER=1.

C TYPE 334

C 334 FORMAT(5X,'NO CONVERGENCE.MAXIMUM NUMBER OF ITERATIONS USED.')

IF(IPRINT.NE.1) GOTO 800

WRITE(ND,1753)

1763 FORMAT(5X,'FUNCTION VALUES AT THE LAST APPROXIMATION FOLLOW:')

C TYPE 335

C 335 FORMAT(5X,'FUNCTION VALUES AT THE LAST APPROXIMATION FOLLOW:')

IFLAG = 1

GOTO 7777

725 IF(IPRINT.NE.1) GOTO 800

C OPEN(UNIT=ND,DEVICE='DSK')

7777 DO 750 K = 1,N

CALL AUXFCN(X,PART(K),K)

750 CONTINUE

IF(IFLAG.NE.1) GOTO 8777

WRITE(ND,7788) (PART(K),K = 1,N)

7788 FORMAT(6E20.8)

C TYPE 336, (PART(K),K=1,N)

C 336 FORMAT(6E20.8)

GOTO 800

8777 WRITE(ND,751)

751 FORMAT(//'CONVERGENCE HAS BEEN ACHIEVED.THE FUNCTION VALUES.')

WRITE(ND,7515) (PART(K),K = 1,N)

7515 FORMAT(5X,'AT THE FINAL APPROXIMATION FOLLOW://(6E20.8)/')

ASTER=2.

C TYPE 337

C 337 FORMAT(//'CONVERGENCE HAS BEEN ACHIEVED.THE FUNCTION VALUES.')

C TYPE 338, (PART(K),K=1,N)

C 338 FORMAT(5X,'AT THE FINAL APPROXIMATION FOLLOW://(6E20.8)/')

GOTO 800

775 CONTINUE

C OPEN(UNIT=ND,DEVICE='DSK')

WRITE(ND,752)

752 FORMAT(//5X,'MODIFIED JACOBIAN IS SINGULAR.TRY A DIFFERENT')

WRITE(ND,7525)

7525 FORMAT(5X,'INITIAL APPROXIMATION.')

ASTER=3.

C TYPE 339

C 339 FORMAT(//5X,'MODIFIED JACOBIAN IS SINGULAR.TRY A DIFFERENT')

C TYPE 401

401 FORMAT(5X,'INITIAL APPROXIMATION.')

800 MAXIT = M+1


```
CLOSE(UNIT=ND,DEVICE='DSK')
RETURN
END
```

```
SUBROUTINE BACK(KMIN,N,X,ISUB,CDE,LOOKUP)
```

This subroutine back-solves the first KMIN rows of a triangularized linear system for improved X values in terms of previous ones.

```
DIMENSION X(30),CDE(30,31)
DIMENSION ISUB(30),LOOKUP(30,31)
DO 200 KK = 1,KMIN
  KM = KMIN-KK+2
  KMAX = ISUB(KM-1)
  X(KMAX) = 0.0E+00
  DO 100 J=KM,N
    JSUB=LOOKUP(KM,J)
    X(KMAX)=X(KMAX)+CDE(KM-1,JSUB)*X(JSUB)
  CONTINUE
  X(KMAX) = X(KMAX)+CDE(KM-1,N+1)
  CONTINUE
  RETURN
END
```

```
SUBROUTINE AUXFON(X,Y,K)
```

```
DIMENSION X(30)
COMMON FO,AK,AKA,AKI,AKLA,AKI,AKS,SXS,SCX,SMX,V,VG,H40,AKT,SP,
1 P,CX0,CS0,CC0,CZ0,CT0
CX=X(1)
CS=X(2)
CC=X(3)
PC=X(4)
CH0=CZ0-CS0
CH=CZ0-CS
CHS=AKI*CC*CS/(AKA*(CZ0-CS))
AMU=H40/(1+AKS/CHS+CHS/AKI)
CONTINUE
GO TO (1,2,3,4),K
Y=FO*(CX0-CX)/V+AMU+CX-AKI*CT0
RETURN
Y=FO*(CS0-CS)/V-AMU+CX/SXS
RETURN
Y=FO*(CC0-CC)/V+AMU+CX*SCX+FO*(CH0-CH)/V+
1 AKLA*(AK*PC-CC)
RETURN
Y=-P*SP*V*AKLA*(AK*PC-CC)/VG-PC*(SP*V*SMX+AMU+CX-
1 SP*V*AKLA*(AK*PC-CC))/VG
RETURN
END
```

APPENDIX B.2 =====

THIS PROGRAM COMPUTES 20 RELATIVE GAIN ARRAYS AT A STEADY
STATE AND AT A PARTICULAR FLOW RATE.

PROGRAM SOLVE;

```

const
  M=4;N=3;K1=0.1E-5;KA=0.316E-4;CZ0=0.1;HMO=0.4;
  KS=0.333E-4;R1=1.0E-5;SP=25.5;V=10.0;SMA=47.0;
type
  MATRIX=array [1..N,1..N] of real;
  FMATRIX=array [1..M,1..N] of real;
var
  DCX0,DCS0,DCC0,CS,CC,PC,CX,CHS,MU:real;
  I,J:integer;
  OBSVAR=array [2..7,1..6] of real;
  IMATRIX=array [1..6,1..N] of real;

```

(MATINV INVERTS A MATRIX A, OF ORDER N AND THE INVERSED
MATRIX IS CALLED C.)

```

procedure MATINV(A:MATRIX;N:integer;var C:MATRIX);
var

```

```

  I,J,K:integer;
  X:real;
begin
  for I:=1 to N do
    for J:=1 to N do
      if I=J then C[I,J]:=1
      else C[I,J]:=0;
    for I:=1 to N do
      begin
        X:=A[I,I];
        for J:=1 to N do
          begin
            A[I,J]:=A[I,J]/X;
            C[I,J]:=C[I,J]/X;
          end;
        for J:=1 to N do
          begin
            X:=A[J,I];
            if I<>J then
              for K:=1 to N do
                begin
                  A[J,K]:=A[J,K]-A[I,K]*X;
                  C[J,K]:=C[J,K]-C[I,K]*X;
                end
              end
            end
          end
        end;
      end;
    end;
  end;
end;

```

[FOUR-TRI FORMS ALL POSSIBLE 3*3 MATRICES FROM THE 4*3 MATRIX
'IMATRIX'. ALL OF THESE ARE STORED IN A 4*3*3 ARRAY 'GMATRIX'.
EACH OF THESE MATRICES IS INVERTED. (INVERSED MATRICES
TOGETHER FORM 'GIMAT'). THEN TRANSPOSE OF EACH INVERTED MATRIX
IS MULTIPLIED BY THE CORRESPONDING ORIGINAL MATRIX.]

```

PROCEDURE FOUR_TRI(IMATRIX:FMATRIX);

```

```

var J,I,K:integer;
    FROW:boolean;
    GMATRIX,GIMAT:array [1..M,1..P,1..N] of real;
    TEMP,TEMP1:MATRIX;
begin
  for I:=1 to M do
    begin
      FROW:=false;
      for J:=1 to N do
        begin
          L:=J;
          if (L=I) then FROW:=true;
          if (FROW=true) then L:=L+1;
          for K:=1 to N do
            GMATRIX[I,J,K]:=IMATRIX[I,K];
          end;
        end;
      end;
    for I:=1 to M do
      begin
        for J:=1 to N do
          for K:=1 to N do
            TEMP[J,K]:=GMATRIX[I,J,K];
          end;
        for J:=1 to N do
          begin
            for K:=1 to N do
              end;
            MATINV(TEMP,N,TEMP);
            for J:=1 to N do
              begin
                for K:=1 to N do
                  begin
                    GIMAT[I,J,K]:=TEMP[J,K];
                  end;
                end;
              end;
            end;
          end;
        for I:=1 to M do
          begin
            WRITELN;WRITELN('LAMBDA ',I);WRITELN;
            for J:=1 to N do
              begin
                for K:=1 to N do
                  begin
                    TEMP1[J,K]:=GMATRIX[I,J,K]*GIMAT[I,K,J];
                    WRITE(TEMP1[J,K]);
                  end;
                end;
              end;
            end;
          end;
        end;
      end;
    end;
  end;
end;

```

[GIVEN FOUR INTEGERS I,J,K AND L, 'SELECT' FORMS A 4*4 MATRIX. MAT
 GOT FROM THE ITH,JTH,KTH,AND LTH ROWS OF 'IMATRIX'. HERE FOUR-101
 IS CALLED WITH 'MAT' AS THE PARAMETER.]

```

procedure select(i,j,k,l:integer);
var
  MAT:FMATIX;
  M,P,Q:INTEGER;
begin

```

```

      Q:=1;
    for M:=1 to 6 do
if (M=I) or (M=J) or (M=K) or (M=L)
      then
begin
  for P:=1 to N do
    MAT[Q,P]:=IMATRIX[M,P];
  Q:=Q+1
end;
  WRITELN('OUTPUT FOR-',I:2,J:2,K:2,L:2);
  WRITELN;
  FOUR_TRI(MAT)
end;

[IMATRIX[I,J] GIVES THE RATE OF CHANGE OF Ith OBSERVED VARIABLE
WITH RESPECT TO THE Jth CONTROLLED VARIABLE.]

begin
  READ(DCX0,DCS0,DCC0);
  for I:=2 to 7 do
    begin
      for J:=1 to 4 do READ(OBSVAR[1,J]);
      CX:=OBSVAR[1,1];
      CS:=OBSVAR[1,2];
      CC:=OBSVAR[1,3];
      PC:=OBSVAR[1,4];
      CHS:=K1*CC*CS/(KA*(CZ0-CS));
      MU:=4MU/(1+KS/CHS+CHS/K1);
      OBSVAR[1,5]:=SP*V*SAX*MU*CX;
      OBSVAR[1,6]:=-LOG(K1*CC/(CZ0-CS));
      READLN
    end;
  for I:=1 to 6 do
    begin
      IMATRIX[I,1]:=(OBSVAR[2,I]-OBSVAR[3,I])/DCX0;
      IMATRIX[I,2]:=(OBSVAR[4,I]-OBSVAR[5,I])/DCS0;
      IMATRIX[I,3]:=(OBSVAR[6,I]-OBSVAR[7,I])/DCC0;
    end;
  for I:=1 to 6 do
    begin
      for J:=1 to N do
        WRITE(IMATRIX[I,J]);
      WRITELN
    end;
  WRITELN;WRITELN;
  SELECT (1,2,3,4);
  SELECT (1,2,5,6);
  SELECT (3,4,5,6);
  SELECT (1,3,5,6);
  SELECT (1,4,5,6);
  SELECT (2,3,5,6);
  SELECT (2,4,5,6);
end.

```

APPENDIX B.3

PROGRAM FOR DYNAMIC SIMULATION WITH TIMELAG
=====

DIMENSION OBSVAR(6), OBSVA1(6), W(6,30), JVAR(6,100), VCHS(10)
THE PARAMETERS USED ARE

FO=FLOW RATE, L/DAY.
AK=HENRY'S LAW CONSTANT, MOL/L ATM.
AKA=ACID DISSOCIATION CONSTANT, MOL/L.
AKI=INHIBITION CONSTANT, MOL/L.
AKLA=OVERALL GAS TRANSFER FILM COEFF, /DAY.
AK1=IONISATION CONSTANT OF BICARBONATE, MOL/L.
AKS=SATURATION CONSTANT, MOL/L.
SXS=ORGANISM YIELD.
SCX=CO2 YIELD.
SMX=CH4 YIELD.
V=DIGESTER LIQUID VOLUME, L.
VG=VOLUME OF GAS SPACE, L.
HMO=MAX. SPECIFIC GROWTH RATE, /DAY.
AKT=TOXICITY INFLUENCE RATE, /DAY.
SP=CONVERSION FACTOR, L/MOL.
P=TOTAL PRESSURE, ATM.
CX0, CS0, CC0, CZ0, CT0=INLET CONCENTRATIONS OF ORGANISMS, LIMITING
SUBSTRATE, DISSOLVED CO2, NET CATION AND TOXIC COMPOUNDS RESPECTIVELY

DATA FO, AK, AKA, AKI, AKLA, AK1, AFS, SYS, SCA, SMA, V, VG, HMO, AKT, SXS,
CX0, CS0, CC0, CZ0, CT0, 1.0, 0.024593, 0.316E-4, 1.0E-5, 30.0, 0.1E-3,
0.333E-4, 0.02, 47.0, 10.0, 2.0, 0.4, 2.0, 25.0, 0.93421, 0.001,
0.09, 0.009, 0.1, 0.0/
COMMON FO, AK, AKA, AKI, AKLA, AK1, AFS, SXS, SCX, SMA, V, VG, HMO, AKT,
SP, P, CX0, CS0, CC0, CZ0, CT0, CHS, AMU
EXTERNAL FCN

N=6
IW=30
READ(5,*)TOL
IFAIL=0
TIME1=0.0
READ(21,*) TL, DTIME
READ(21,*)(OBSVAR(I), I=1,6)
DO 5 I=1,6
OBSVA1(I)=OBSVAR(I)
M1=TL/DTIME
HERE TL=TIME LAG, DTIME=INCREMENT.
TYPE *, TL, DTIME, M1
CS=OBSVA1(2)
CC=OBSVA1(3)
CZ=OBSVA1(5)
CHS=AK1*CC*CS/(AKA*(CZ-CS))
AMU=HMO/(1+AKS/CHS+CHS/AK1)
INTEGRATION IS DONE FROM 0.0 TO TL
VALUES OF CHS OBTAINED ARE STORED IN VCHS(N).
DO 10 I=1, M1
CS=OBSVA1(2)
CC=OBSVA1(3)
CZ=OBSVA1(5)
CHS=AK1*CC*CS/(AKA*(CZ-CS))
TIME=TIME1+DTIME
NAG ROUTINE D02EAF INTEGRATES A STIFF SYSTEM OF DIFFERENTIAL

EQUATIONS OVER A RANGE, WITH SUITABLE INITIAL CONDITIONS,
USING THE VARIABLE-ORDER, VARIABLE-STEP GEAR METHOD.
HERE D02EAF INTEGRATES FCN BETWEEN TIME1 AND TIME.
OBSVA1 IS OF SIZE N.

```

CALL D02EAF (TIME1, TIME, N, OBSVA1, TOL, FCN, W, IN, IFAIL)
CALL OUT(TIME1, OBSVA1)
VCHS(1)=CHS
TYPE*, TIME1
TYPE *, (OBSVA1(J), J=1, 6)
CONTINUE
READ(21, *) FTIME
M=(FTIME-TL)/DTIME
DO 20 I=1, M
CHS=VCHS(1)
AMU=HMU/(1+AKS/CHS+CHS/AKI)
IF (MOD(I, 10) .NE. 0) GOTO 60
CALL OUT(TIME1, OBSVA1)
TIME=TIME1+DTIME
INTEGRATION IS DONE BETWEEN TIME1 AND TIME, WITH THE VALUE
OF CHS LAGGING. CHS IS CHOSEN AS VCHS(1) AND VCHS IS READJUSTED.
CALL D02EAF(TIME1, TIME, N, OBSVA1, TOL, FCN, W, IN, IFAIL)
DO 30 J=1, (M1-1)
VCHS(J)=VCHS(J+1)
CS=OBSVA1(2)
CC=OBSVA1(3)
CZ=OBSVA1(5)
VCHS(M1)=AK1*CC*CS/(AKA*(CZ-CS))
CONTINUE
STOP
END
FCN COMPUTES THE FUNCTION F FOR THE VALUES OF VARIABLES
CONTAINED IN OBSVAR.
SUBROUTINE FCN(I, OBSVAR, F)
DIMENSION OBSVAR(6), F(6)
COMMON FO, AK, AKA, AKI, AKLA, AK1, AKS, SXS, SCX, SXX, V, VG, HMU, AK1,
1 SP, P, CX0, CS0, CC0, CZ0, CT0, CHS, AMU
IF (T .GT. 1.0) FO=1.0
CX=OBSVAR(1)
CS=OBSVAR(2)
CC=OBSVAR(3)
PC=OBSVAR(4)
CZ=OBSVAR(5)
CT=OBSVAR(6)
CH0=CZ0-CS0
CH=CZ-CS
F(1)=FO*(CX0-CX)/V+AMU*CX-AKT*CT
F(2)=FO*(CS0-CS)/V-AMU*CX/SXS
F(4)=-P*SP*V*AKLA*(AK*PC-CC)/VG-PC*(SP*V*SXX*AMU*CX-
1 SP*V*AKLA*(AK*PC-CC))/VG
F(5)=FO*(CZ0-CZ)/V
F(6)=FO*(CT0-CT)/V
F(3)=FO*(CC0-CC)/V+AMU*CX*SCX+FO*(CH0-CH)/V+F(2)-F(5)+
1 AKLA*(AK*PC-CC)
WRITE(24, *), (F(I), I=1, 6)
RETURN
END
OUTPUT SUBROUTINE.
SUBROUTINE OUT(TIME, OBSVAR)
DIMENSION OBSVAR(6)
COMMON FO, AK, AKA, AKI, AKLA, AK1, AKS, SXS, SCX, SXX, V, VG, HMU, AK1, SP, P,

```

```

1  CX0,CS0,CC0,CZ0,CT0,CHS,AMU
   WRITE (22,*) TIME
5  FORMAT('AT TIME=',F10.5)
   WRITE (22,*)(OBSVAR(I),I=1,6)
   TYPE 10,TIME
10  FORMAT(/5X,F10.4)
   TYPE *,(OBSVAR(I),I=1,6)
   PCO2=OBSVAR(4)/P*100
   OCH4=SP*V*SMX*AMU*OBSVAR(1)
   HCO3=OBSVAR(5)-OBSVAR(2)
   PH=-ALOG10(AK1*OBSVAR(3)/HCO3)
   WRITE(24,*) TIME
6  FORMAT('AT TIME=',F10.5)
50  WRITE (24,*) PCO2,CHS,AMU,OCH4,HCO3,PH
   TYPE *,PCO2,CHS,AMU,OCH4,HCO3,PH
   RETURN
   END

```